

10/672412

=> file registry

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DICTIONARY FILE UPDATES: 26 JUN 2007 HIGHEST RN 939408-72-7

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<http://www.cas.org/support/stngen/stndoc/properties.html>

=> file zcaplus

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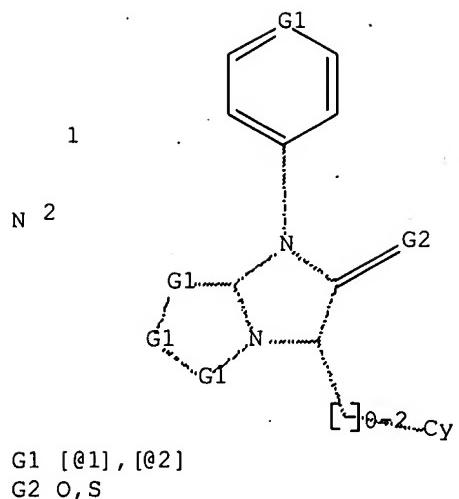
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FILE COVERS 1907 - 27 Jun 2007 VOL 147 ISS 1
FILE LAST UPDATED: 26 Jun 2007 (20070626/ED)

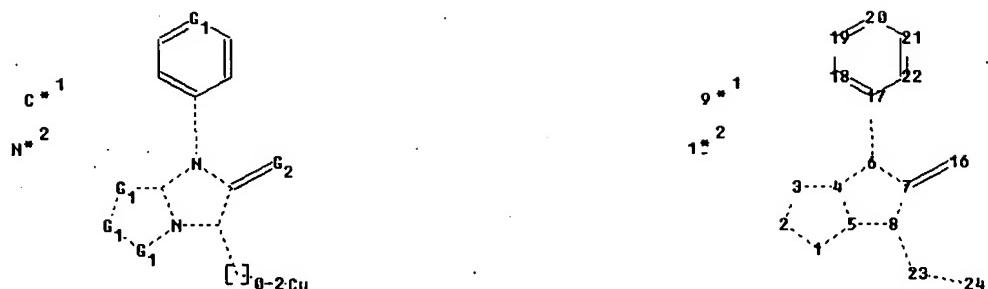
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'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPPLUS' FILE

=> d stat que L23
L1 STR



Structure attributes must be viewed using STN Express query preparation:
 Uploading L1.str



chain nodes :

16 23 24

ring nodes :

1 2 3 4 5 6 7 8 9 10 17 18 19 20 21 22

chain bonds :

6-17 7-16 8-23 23-24

ring bonds :

1-2 1-5 2-3 3-4 4-5 4-6 5-8 6-7 7-8 17-18 17-22 18-19 19-20 20-21 21-22

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5 4-6 5-8 6-7 6-17 7-8 7-16 8-23 17-18 17-22 18-19
19-20 20-21 21-22 23-24

G1:[*1], [*2]

G2:O,S

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS 24:Atom

Generic attributes :

24:

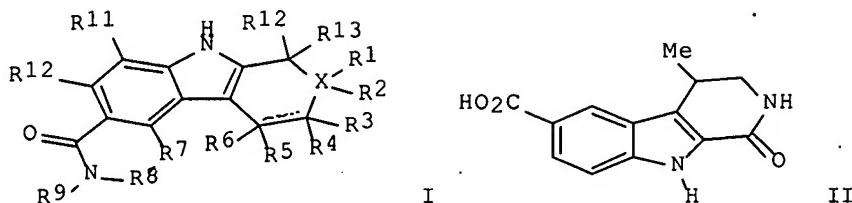
Saturation : Unsaturated

L4	22734 SEA FILE=ZCPLUS ABB=ON	PLU=ON	WU J?/AU
L5	1187 SEA FILE=ZCPLUS ABB=ON	PLU=ON	KELLY T?/AU
L6	419 SEA FILE=ZCPLUS ABB=ON	PLU=ON	LEMIEUX R?/AU
L7	1095 SEA FILE=ZCPLUS ABB=ON	PLU=ON	GOLDBERG D?/AU
L8	8 SEA FILE=ZCPLUS ABB=ON	PLU=ON	EMEIGH J?/AU
L9	21 SEA FILE=ZCPLUS ABB=ON	PLU=ON	SORCEK R?/AU
L10	16 SEA FILE=ZCPLUS ABB=ON	PLU=ON	L4 AND (L5 OR L6 OR L7 OR L8 OR L9)
L11	11 SEA FILE=ZCPLUS ABB=ON	PLU=ON	L5 AND (L6 OR L7 OR L8 OR L9)
L12	2 SEA FILE=ZCPLUS ABB=ON	PLU=ON	L6 AND (L7 OR L8 OR L9)
L13	2 SEA FILE=ZCPLUS ABB=ON	PLU=ON	L7 AND (L8 OR L9)
L14	3 SEA FILE=ZCPLUS ABB=ON	PLU=ON	L8 AND L9
L15	22 SEA FILE=ZCPLUS ABB=ON	PLU=ON	(L10 OR L11 OR L12 OR L13 OR L14)
L19	572 SEA FILE=REGISTRY SSS FUL L1		
L20	28 SEA FILE=ZCPLUS ABB=ON	PLU=ON	L19
L22	7 SEA FILE=ZCPLUS ABB=ON	PLU=ON	(L4 OR L5 OR L6 OR L7 OR L8 OR L9) AND L20
L23	23 SEA FILE=ZCPLUS ABB=ON	PLU=ON	L15 OR L22

=> d ibib abs hitind L23 1-23

L23 ANSWER 1 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1286266 ZCPLUS Full-text
DOCUMENT NUMBER: 146:45497
TITLE: Anti-cytokine heterocyclic compounds as MAPKAP-K2
inhibitors and their preparation, pharmaceutical
compositions and use in the treatment of diseases
INVENTOR(S): *Goldberg, Daniel; Abeywardane, Asitha;
Miller, Craig; Morwick, Tina; Netherton, Matthew;
Snow, Roger; Wang, Ji; Wu, Jiang-Ping;
Xiong, Zhaoming*
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 82pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006276496	A1	20061207	US 2006-276933 US 2005-662936P US 2005-719164P	20060317 P 20050317 P 20050921
PRIORITY APPLN. INFO.:				
OTHER SOURCE(S): GI	MARPAT 146:45497			



AB Heterocyclic compds. of formula I and analogs thereof and their use as inhibitors of Mitogen-Activated Protein Kinase-Activated Protein kinase-2 (MAPKAP-k2), and also to a method for preventing or treating a disease or disorder that can be treated or prevented by modulating the activity of MAPKAP-K2 in a subject and to pharmaceutical compns. and kits that include these MAPKAP-K2 inhibitors. Compds. of formula I wherein X is C and N; R1 is H, OH, carbamoyl, C1-6 alkyl, C2-6 alkenyl(oxy), C2-6 alkynyl(oxy), C1-6 alkoxy, etc.; R2 is absent, H, OH, ureido, C1-6 alkyl, C2-6 alkenyl(oxy), C2-6 alkynyl(oxy), C1-6 alkoxy, etc.; R3 is H, amino, C1-6 alkyl(amino), C2-6 alkenyl(oxy), C2-6 alkynyl, etc.; R4 is absent, H, amino, C1-6 alkyl(amino), C2-6 alkenyl, CN, C1-6 alkynyl, etc.; R5 is absent, H, oxo, C1-6 (halo)alkyl, C2-6 alkenyl(oxy), C2-6 alkynyl(oxy), C1-6 alkoxy, OH, etc.; R6 is H, oxo, C1-6 (halo)alkyl, C2-6 alkenyl(oxy), C2-6 alkynyl(oxy), OH, C3-7 cycloalkyl, etc.; R7 is H, C1-6 alkyl, C3-7 cycloalkyl, C1-6 alkoxy, OH, etc.; R8 is H, C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, C1-6 alkoxy, and C3-7 cycloalkyl; R9 is H, halo, C1-6 alkyl, C2-6 alkenyl(oxy), C2-6 alkynyl(oxy), C1-6 alkoxy, etc.; R10 and R11 are independently H, C1-6 alkoxy, OH, halo, C1-6 alkyl, and C3-7 cycloalkyl; R12 is =S, =O, C1-6 alkyl, CN, aminoalkyl, amino, haloalkyl, etc.; R13 is absent, H, C1-6 alkyl, and halo; and their pharmaceutically acceptable salts are claimed. Example compound II was prepared by conjugate addition of di-Et malonate to methacrylonitrile; the resulting 2-(2-cyano-2-methylethyl)malonic acid di-Et ester underwent cyclization to give 5-methyl-2-oxopiperidine-3-carboxylic acid Et ester, which underwent condensation with sodium nitrite and 4-aminobenzoic acid Et ester to give 4-[N'-(5-methyl-2-oxopiperidin-3-ylidene)hydrazino]benzoic acid Et ester, which underwent cyclization to give 4-methyl-1-oxo-2,3,4,9-tetrahydro-1H-β-carboline-6-carboxylic acid Et ester, which underwent hydrolysis to give compound II. All the invention compds. were evaluated or their MAPKAP-K2 inhibitory activity.

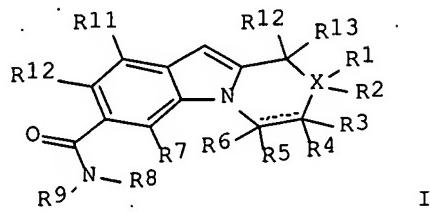
INCL 514291000; 514411000; 548444000; 546085000

CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

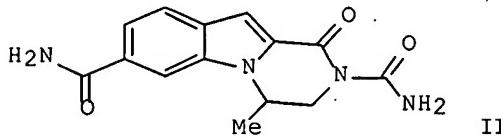
L23 ANSWER 2 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1286238 ZCPLUS Full-text
DOCUMENT NUMBER: 146:45542
TITLE: Anti-cytokine heterocyclic compounds as MAPKAP-K2

INVENTOR(S): inhibitors and their preparation, pharmaceutical
 compositions and use in the treatment of diseases
Goldberg, Daniel; Abeywardane, Asitha;
Miller, Craig; Morwick, Tina; Netherton, Matthew;
Snow, Roger; Wang, Ji; Wu, Jiang-Ping;
Xiong, Zhaoming
 PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
 SOURCE: U.S. Pat. Appl. Publ., 50pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006276453	A1	20061207	US 2006-276935	20060317
PRIORITY APPLN. INFO.:			US 2005-662567P	P 20050317
			US 2005-719017P	P 20050921
OTHER SOURCE(S):	MARPAT 146:45542			
GI				



I



II

AB Heterocyclic compds. of formula I and analogs thereof and their use as
 inhibitors of Mitogen-Activated Protein Kinase-Activating Protein kinase-2
 (MAPKAP-K2), and also to a method for preventing or treating a disease or
 disorder that can be treated or prevented by modulating the activity of
 MAPKAP-K2 in a subject and to pharmaceutical compns. and kits that include
 these MAPKAP-K2 inhibitors. Compds. of formula I wherein X is C and N; R1 is
 H, OH, carbamoyl, C1-6 alkyl, C2-6 alkenyl(oxy), C2-6 alkynyl(oxy), C1-6
 alkoxy, etc.; R2 is absent, H, OH, ureido, C1-6 alkyl, C2-6 alkenyl(oxy), C2-6
 alkynyl(oxy), C1-6 alkoxy, etc.; R3 is H, amino, C1-6 alkyl(amino), C2-6
 alkenyl(oxy), C2-6 alkynyl, etc.; R4 is absent, H, amino, C1-6
 alkyl(amino), C2-6 alkenyl, CN, C1-6 alkynyl, etc.; R5 is absent, H, oxo,
 C1-6 (halo)alkyl, C2-6 alkenyl(oxy), C2-6 alkynyl(oxy), C1-6 alkoxy, OH, etc.;
 R6 is H, oxo, C1-6 (halo)alkyl, C2-6 alkenyl(oxy), C2-6 alkynyl(oxy), OH, C3-7
 cycloalkyl, etc.; R7 is H, C1-6 alkyl, C3-7 cycloalkyl, C1-6 alkoxy, OH, etc.;
 R8 is H, C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, C1-6 alkoxy, and C3-7
 cycloalkyl; R9 is H, halo, C1-6 alkyl, C2-6 alkenyl(oxy), C2-6 alkynyl(oxy),
 C1-6 alkoxy, etc.; R10 and R11 are independently H, C1-6 alkoxy, OH, halo, C1-

6 alkyl, and C3-7 cycloalkyl; R12 is =S, =O, C1-6 alkyl, CN, aminoalkyl, amino, haloalkyl, etc.; R13 is absent, H, C1-6 alkyl, and halo; and their pharmaceutically acceptable salts are claimed. Example compound II was prepared by amidation of 4-methyl-1-oxo-1,2,3,4-tetrahydropyrazino[1,2-a]indole-7-carboxylic acid followed by carbamoylation with Ghosez's reagent. All the invention compds. were evaluated or their MAPKAP-K2 inhibitory activity.

INCL 514214010; 514220000; 514250000; 514291000; 544344000; 540558000;
540586000

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

L23 ANSWER 3 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1225839 ZCPLUS Full-text

DOCUMENT NUMBER: 146:7960

TITLE: Derivatives of 6,7-dihydro-5H-imidazo[1,2-a]imidazole-3-sulfonic acid and their preparation, pharmaceutical compositions, and their inhibitory activity upon interaction of CAMs and leukointegrins and use in the treatment of inflammatory diseases

INVENTOR(S): Barry, John Patrick; Eriksson, Magnus Carl Arne;
Joseph, David P.; Lemieux, Rene' Marc; Wang,
Xiao-Jun

PATENT ASSIGNEE(S): Boehringer Ingelheim International GmbH, Germany

SOURCE: U.S. Pat. Appl. Publ., 30pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006264472	A1	20061123	US 2006-382940	20060512
WO 2007027233	A2	20070308	WO 2006-US16903	20060503
WO 2007027233	A3	20070426		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				

PRIORITY APPLN. INFO.: US 2005-682462P P 20050519

OTHER SOURCE(S): MARPAT 146:7960

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Derivs. of 6,7-dihydro-5H-imidazo[1,2-a]imidazole-3-sulfonic acid of formula I, which exhibit good inhibitory effect upon the interaction of CAMs and Leukointegrins and are thus useful in the treatment of inflammatory disease.

Compds. of formula I wherein R1 is OH and NH2; R2 is (un)substituted pyridinyl, (un)substituted pyrimidinyl, CN, halo, NH2 and derivs., and OCF3; R3 is (un)branched C1-3 alkyl; each R4 are independently halo, C1-2 haloalkyl; X is CH=, N=; Y is O and S; and their pharmaceutically acceptable salts thereof are claimed. Example compound II was prepared by iodination of (R)-3-(4-bromobenzyl)-1-(3,5-dichlorophenyl)-3-methyl-1H-imidazo[1,2-a]imidazol-2-one followed by sulfonylation; the resulting imidazo[1,2-a]imidazolesulfonyl chloride underwent hydrolysis to give the corresponding (4-bromobenzyl)imidazo[1,2-a]imidazole-3-sulfonic acid, which underwent boration with bispinacloato diboron to give the corresponding arylborate which underwent cross coupling with 4-amino-5-bromopyrimidine to give compound II. All the invention compds. were evaluated for their inhibition of LFA-1 binding to ICAM-1. From the assay, it was determined that the tested compds. exhibited Kd values of < 10 μM.

INCL 514338000; 514393000; 546273100; 548303100

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 63

IT 915385-21-6P 915385-22-7P 915385-23-8P

915385-24-9P 915385-25-0P 915385-26-1P

915385-30-7P 915385-31-8P 915385-32-9P

915385-33-0P 915385-34-1P 915385-35-2P

915385-36-3P 915385-37-4P 915385-38-5P

915385-39-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of dihydroimidazoimidazolesulfonic acid derivs. and their inhibitory activity upon interaction of CAMs and leukointegrins and use in the treatment of inflammatory diseases)

IT 1439-10-7, 4-Amino-5-bromopyrimidine 73183-34-3 321656-72-8
688756-17-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of dihydroimidazoimidazolesulfonic acid derivs. and their inhibitory activity upon interaction of CAMs and leukointegrins and use in the treatment of inflammatory diseases)

IT 321657-06-1P 321657-07-2P 321719-03-3P
321721-20-4P 321724-08-7P 688756-08-3P
688756-18-5P 688756-19-6P 915385-27-2P
915385-28-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of dihydroimidazoimidazolesulfonic acid derivs. and their inhibitory activity upon interaction of CAMs and leukointegrins and use in the treatment of inflammatory diseases)

L23 ANSWER 4 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:357148 ZCPLUS Full-text

DOCUMENT NUMBER: 145:39831

TITLE: Evolution of the Thienopyridine Class of Inhibitors of IKB Kinase-β: Part I: Hit-to-Lead Strategies

AUTHOR(S): Morwick, Tina; Berry, Angela; Brickwood, Janice;
Cardozo, Mario; Catron, Katrina; DeTuri, Molly;
Emeigh, Jonathan; Homon, Carol; Hrapchak,
Matt; Jacober, Stephen; Jakes, Scott; Kaplita, Paul;
Kelly, Terence A.; Ksiazek, John; Liuzzi,
Michel; Magolda, Ronald; Mao, Can; Marshall, Daniel;
McNeil, Daniel; Prokopowicz, Anthony, III; Sarko,
Christopher; Scouten, Erika; Sledziona, Cynthia; Sun,
Sanxing; Watrous, Jane; Wu, Jiang Ping;

CORPORATE SOURCE: Cywin, Charles L.
Boehringer Ingelheim Pharmaceuticals, Inc.,
Ridgefield, CT, 06801-0368, USA
SOURCE: Journal of Medicinal Chemistry (2006), 49(10),
2898-2908
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:39831

AB High-throughput screening is routinely employed as a method for the identification of novel hit structures. Large nos. of active compds. are typically procured in this way and must undergo a rigorous validation process. This process is described in detail for a collection of screening hits identified as inhibitors of I κ B kinase- β (IKK β), a key regulatory enzyme in the nuclear factor- κ B (NF- κ B) pathway. From these studies, a promising hit series was selected. Subsequent lead generation activities included the development of a pharmacophore hypothesis and structure-activity relationship (SAR) for the hit series. This led to the exploration of related scaffolds offering addnl. opportunities, and the various structural classes were comparatively evaluated for enzyme inhibition, selectivity, and drug-like properties. A novel lead series of thienopyridines was thereby established, and this series advanced into lead optimization for further development.

CC 1-3 (Pharmacology)
REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 5 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:229064 ZCAPLUS Full-text
DOCUMENT NUMBER: 144:343275
TITLE: An orally active, primate selective antagonist of LFA-1 inhibits delayed-type hypersensitivity in a humanized-mouse model
AUTHOR(S): Panzenbeck, Maret J.; Jeanfavre, Deborah D.; Kelly, Terence A.; Lemieux, Rene; Nabozny, Gerald; Reilly, Patricia L.; Desai, Sudha
CORPORATE SOURCE: Department of Immunology and Inflammation, Boehringer Ingelheim Pharmaceutical Inc., Ridgefield, CT, 06877-0368, USA
SOURCE: European Journal of Pharmacology (2006), 534(1-3), 233-240
PUBLISHER: CODEN: EJPHAZ; ISSN: 0014-2999
DOCUMENT TYPE: Elsevier B.V.
LANGUAGE: Journal
English

AB Compound I, a novel small mol. antagonist ($K_d = 6$ nM) of human lymphocyte function-associated antigen-1 (LFA-1, CD11a/CD18) was tested for activity in a humanized mouse model of delayed-type hypersensitivity (trans vivo delayed-type hypersensitivity). Trans vivo delayed-type hypersensitivity is a model for testing compds. with human targets in mice. Tetanus toxoid and 7-10 + 106 human peripheral blood mononuclear cells from tetanus-sensitized donors were coinjected into footpads of naive mice. Footpads were measured before and 24 h later. Injection of peripheral blood mononuclear cells plus antigen resulted in swelling of 0.178-0.254 mm, significantly greater than peripheral blood mononuclear cells or tetanus toxoid alone ($P < 0.05$). Preincubation of peripheral blood mononuclear cells with anti-human major histocompatibility complex class II (MHCII) or anti-human LFA-1 monoclonal antibody (mAb), but not anti-mouse MHCII or anti-mouse LFA-1 mAb, significantly inhibited the response. Compound I inhibited footpad swelling in a dose related manner (0.1-100 mg/kg, p.o.; ED50 apprx. 1 mg/kg), whereas its enantiomer had no

effect. These data demonstrate the oral efficacy of a novel antagonist of LFA-1 in trans vivo delayed-type hypersensitivity.

CC 1-7 (Pharmacology)
IT 321656-63-7

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(LFA-1 antagonist activity in delayed-type hypersensitivity)

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 6 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:168805 ZCPLUS Full-text
DOCUMENT NUMBER: 142:410694
TITLE: Alkylation of Magnesium Sulfinate: A Direct Transformation of Functionalized Aromatic/Heteroaromatic Halides into Sulfones
AUTHOR(S): Wu, Jiang-Ping; Emeigh, Jonathan;
Su, Xi-Ping
CORPORATE SOURCE: Department of Medicinal Chemistry, Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT, 06877, USA
SOURCE: Organic Letters (2005), 7(7), 1223-1225
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:410694

AB Sulfinate alkylation is one of the conventional methods for sulfone synthesis. The alkylation of magnesium sulfinate, which are easily accessible via reactions of organomagnesium intermediates with sulfur dioxide, provides a convenient route for sulfone preparation. In this communication, the authors report a preliminary study of the alkylation of arylmagnesium sulfinate. An application of this reaction to directly transform functionalized aromatic/heteroarom. halides into sulfones is also described.

CC 21-2 (General Organic Chemistry)
IT 96-33-3, Methyl acrylate 922-67-8, Methyl propiolate 1120-90-7,
3-Iodopyridine 1521-51-3 4753-59-7, 7446-09-5, Sulfur dioxide,
reactions 16494-36-3 33240-34-5, Cyclopentylmagnesium bromide,
40596-44-9 51934-41-9, Ethyl 4-iodobenzoate 321656-73-9
850425-82-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of sulfones via generation of Grignard reagents from aromatic/heteroarom. halides by magnesium-halide exchange followed by reaction with sulfur dioxide and alkylation of the magnesium sulfinate intermediates)

IT 321723-77-7P 850425-75-1P 850425-76-2P 850425-77-3P
850425-78-4P 850425-81-9P 850425-83-1P 850425-84-2P 850425-85-3P
RL: SPN (Synthetic preparation); PREP, (Préparation)

(preparation of sulfones via generation of Grignard reagents from aromatic/heteroarom. halides by magnesium-halide exchange followed by reaction with sulfur dioxide and alkylation of the magnesium sulfinate intermediates)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 7 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:790832 ZCPLUS Full-text
DOCUMENT NUMBER: 142:6469
TITLE: Second-generation lymphocyte function-associated antigen-1 inhibitors: 1H-imidazo[1,2- α]imidazol-2-one derivatives

AUTHOR(S): *Emeigh, Jonathan; Gao, Donghong A.; Goldberg, Daniel R.; Kuzmich, Daniel; Miao, Clara; Potocki, Ian; Qian, Kevin C.; Sorcek, Ronald J.; Jeanfavre, Deborah D.; Kishimoto, Kei; Mainolfi, Elizabeth A.; Nabozny, Gerald, Jr.; Reilly, Patricia; Rothlein, Robert; Sellati, Rosemarie H.; Woska, Joseph R., Jr.; Chen, Shirlynn; Gunn, Jocelyn A.; O'Brien, Drane; Norris, Stephen H.; Kelly, Terence A.; Peng, Charline; Wu, Jiang-Ping*

CORPORATE SOURCE: Research and Development, Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT, 06877, USA

SOURCE: Journal of Medicinal Chemistry (2004), 47(22), 5356-5366

CODEN: JMCMAR; ISSN: 0022-2623

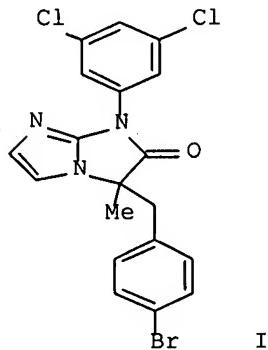
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:6469

GI



AB A novel class of lymphocyte function-associated antigen-1 (LFA-1) inhibitors is described. Discovered during the process to improve the physicochem. and metabolic properties of BIRT377, a previously reported hydantoin-based LFA-1 inhibitor, these compds. are 5- or 6-substituted derivs. of the 1*H*-imidazo[1,2-*a*]imidazol-2-one I. The structure-activity relationship (SAR) shows that electron-withdrawing groups at C(5) on the imidazole ring benefit potency and that oxygen-containing functional groups attached to a C(5)-sulfonyl or sulfonamide group further improve potency. This latter gain in potency is attributed to the interaction(s) of the functionalized sulfonyl/sulfonamide groups with the protein, likely polar-polar in nature, as suggested by SAR data. X-ray studies revealed that these bicyclic inhibitors bind to the I-domain of LFA-1 in a pattern similar to that of BIRT377.

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 1
 IT 321656-72-8P 321719-80-6P 321721-16-8P
 321721-24-8P 321722-24-1P 321723-65-3P
 321723-77-7P
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of 1*H*-imidazo[1,2-*a*]imidazol-2-ones as second-generation

lymphocyte function-associated antigen-1 inhibitors)

IT 321656-35-3P 321656-61-5P 321656-73-9P
 321656-95-5P 321657-00-5P 321657-01-6P
 321657-02-7P 321657-04-9P 321718-99-4P
 321720-06-3P 321720-66-5P 321720-72-3P
 321720-89-2P 321721-28-2P 321722-68-3P
 321722-90-1P 321722-94-5P 321723-35-7P
 321723-54-0P 321723-68-6P 321723-69-7P
 321723-71-1P 321723-75-5P 796871-98-2P
 796871-99-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of 1H-imidazo[1,2- α]imidazol-2-ones as second-generation lymphocyte function-associated antigen-1 inhibitors)

IT 213209-22-4P 321656-74-0P 321656-99-9P 321724-07-6P
 321724-14-5P 321724-15-6P 321724-16-7P 321724-18-9P,
 2-Azidomethyl-1,3-dioxolane 796872-00-9P 796872-01-0P
 796872-02-1P 796872-03-2P 796872-04-3P 797762-16-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 1H-imidazo[1,2- α]imidazol-2-ones as second-generation lymphocyte function-associated antigen-1 inhibitors)

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

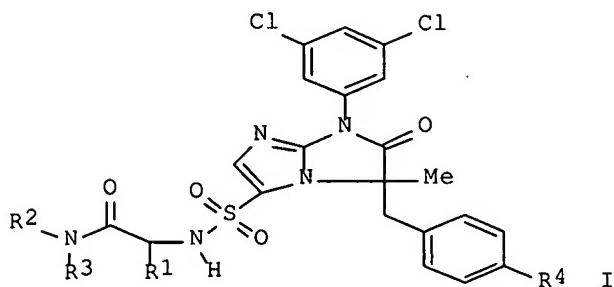
L23 ANSWER 8 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:412950 ZCPLUS Full-text
 DOCUMENT NUMBER: 140:423947
 TITLE: Preparation of [6,7-dihydro-5H-imidazo[1,2-a]imidazole-3-sulfonylamino]propionamide derivatives for treatment of inflammatory disease
 INVENTOR(S): Kelly, Terence Alfred; Kim, Jin Mi;
 Lemieux, Rene Marc
 PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
 SOURCE: PCT Int. Appl., 44 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004041827	A2	20040521	WO 2003-US333865	20031027
WO 2004041827	A3	20040715		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004127534	A1	20040701	US 2003-686073	20031015
US 6844360	B2	20050118		
CA 2504219	A1	20040521	CA 2003-2504219	20031027
AU 2003284938	A1	20040607	AU 2003-284938	20031027
EP 1560830	A2	20050810	EP 2003-779257	20031027

EP 1560830	B1	20061025		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003015836	A	20050913	BR 2003-15836	20031027
CN 1708500	A	20051214	CN 2003-80102491	20031027
JP 2006508947	T	20060316	JP 2004-550109	20031027
EP 1712553	A2	20061018	EP 2006-118540	20031027
EP 1712553	A3	20061102		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, SK				
AT 343582	T	20061115	AT 2003-779257	20031027
NZ 540269	A	20070531	NZ 2003-540269	20031027
US 2005054703	A1	20050310	US 2004-969105	20041020
US 2005165027	A1	20050728	US 2005-34701	20050113
ZA 2005002701	A	20051013	ZA 2005-2701	20050404
NO 2005002579	A	20050527	NO 2005-2579	20050527
PRIORITY APPLN. INFO.:				
			P	20021030
			A3	20031015
			A3	20031027
			W	20031027

OTHER SOURCE(S): MARPAT 140:423947

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AB The invention relates to imidazo[1,2-a]imidazole amino acid derivs. I [R1 is alkyl optionally mono- or disubstituted by oxo or morpholino; R2, R3 are H or alkyl mono- or disubstituted by CONH₂ or OH or R₂R₃N is piperazinyl; R4 is cyano, trifluoromethoxy, pyrimidinyl or mono- or diaminopyrimidinyl] or their pharmaceutically-acceptable salts which exhibit good inhibitory effect upon the interaction of cellular adhesion mols. (CAMs) and leukointegrins and are thus useful in the treatment of inflammatory disease. Thus, I [R₂R₃NCOCHR₁NH is L-alaninamide residue (R ring stereo)] was prepared from (R)-3-(4-bromobenzyl)-1-(3,5-dichlorophenyl)-3-methyl-1H-imidazo[1,2-a]imidazol-2-one by cyanation with Zn(CN)₂, conversion to the sulfonyl chloride (iodination with N-iodosuccinimide, reaction with cyclopentylmagnesium chloride, SO₂ and N-chlorosuccinimide), and condensation with L-alaninamide hydrochloride. Synthesized I showed Kd < 10 μM for inhibition of integrin LFA-1 and ICAM-1.

IC ICM C07D487-04
 ICS A61K031-4164; A61P037-00; C07D235-00
 CC 34-2 (Amino Acids, Peptides, and Proteins)
 Section cross-reference(s): 1, 28, 63
 IT 688755-94-4P 688755-95-5P 688755-96-6P
 688755-97-7P 688755-98-8P 688755-99-9P

688756-00-5P 688756-01-6P 688756-02-7P

688756-03-8P 688756-04-9P 688756-05-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of [(dihydroimidazoimidazolesulfonyl)amino]propionamide derivs.

for treatment of inflammatory disease)

IT 1072-97-5, 5 Bromo 2 pyridinamine 1668-10-6, Glycinamide hydrochloride 6160-65-2, Thiocarbonyldiimidazole 13404-22-3, L-Alanine tert butyl ester hydrochloride 22483-09-6, Aminoacetaldehyde dimethyl acetal 32916-51-1, Cyclopentylmagnesium chloride 33208-99-0, L-Alaninamide hydrochloride 50824-05-0, 4 Trifluoromethoxybenzyl bromide 71810-97-4, D-Alaninamide hydrochloride 73183-34-3 **321656-72-8**
321724-17-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of [(dihydroimidazoimidazolesulfonyl)amino]propionamide derivs.

for treatment of inflammatory disease)

IT 110-91-8P, Morpholine, preparation 30924-93-7P 86150-09-6P
124212-41-5P **321657-06-1P 321657-07-2P**
688756-06-1P 688756-07-2P 688756-08-3P
688756-09-4P 688756-10-7P 688756-11-8P 688756-12-9P
688756-13-0P 688756-14-1P 688756-15-2P 688756-16-3P
688756-17-4P 688756-18-5P 688756-19-6P
689261-01-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of [(dihydroimidazoimidazolesulfonyl)amino]propionamide derivs.

for treatment of inflammatory disease)

L23 ANSWER 9 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:412808 ZCPLUS Full-text

DOCUMENT NUMBER: 140:423673

TITLE: Preparation of derivatives of [6,7-dihydro-5H-imidazo[1,2-a]imidazole-3-sulfonyl]-pyrrolidine-2-carboxylic acid amide as anti-inflammatory agents

INVENTOR(S): Kelly, Terence Alfred; Kim, Jin Mi;
Lemieux, Rene Marc; Tschantz, Matt Aaron

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 98 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

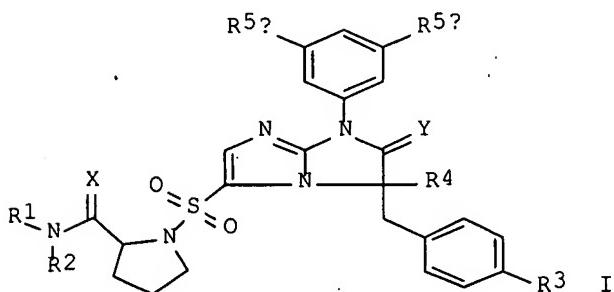
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004041273	A1	20040521	WO 2003-US333966	20031027
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,			

BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
 US 6852748 B1 20050208 US 2003-685638 20031015
 CA 2504131 A1 20040521 CA 2003-2504131 20031027
 AU 2003286700 A1 20040607 AU 2003-286700 20031027
 EP 1558248 A1 20050803 EP 2003-777910 20031027
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
 JP 2006508106 T 20060309 JP 2004-550125 20031027
 US 2005054704 A1 20050310 US 2004-969698 20041020
 PRIORITY APPLN. INFO.: US 2002-422449P P 20021030
 US 2003-685638 A3 20031015
 WO 2003-US33966 W 20031027

OTHER SOURCE(S): MARPAT 140:423673

GI



AB The title compds. [I; R1, R2 = hydrogen (provided that R1 and R2 are not both hydrogen atoms), each (un)substituted straight or branched C1-7 alkyl, C3-6 cycloalkyl, aryl (selected from the group consisting of biphenyl, Ph, or quinolinyl), or unsatd. or partially saturated heterocyclic group containing 2 to 3 C, 1 to 2 N, 0 to 1 S, and 0 to 1 O atoms; or wherein R1 and R2 constitute a saturated 3 to 5-methylene group bridge which together with the nitrogen atom between them form (un)substituted heterocyclic ring; R3 = (un)substituted aryl (selected from the group consisting of pyridyl and pyrimidyl), CF3O, cyano; R4 = straight or branched C1-3 alkyl; R5a, R5b = Cl, CF3; X, Y = O, S; Y] or pharmaceutically acceptable salts thereof are prepared. These compds. exhibit good inhibitory effect upon the interaction of cellular adhesion mols. (CAMs) and leukointegrins and are thus useful in the treatment of inflammatory disease including adult respiratory distress syndrome, shock, oxygen toxicity, multiple organ injury syndrome secondary to septicemia, multiple organ injury syndrome secondary to trauma, reperfusion injury of tissue due to cardiopulmonary bypass, myocardial infarction [associated with use of thrombolysis agents (sic)], acute glomerulonephritis, vasculitis, reactive arthritis, dermatosis with acute inflammatory components, stroke, thermal injury, hemodialysis, leukapheresis, ulcerative colitis, necrotizing enterocolitis, granulocyte transfusion associated syndrome, psoriasis, organ/tissue transplant rejection, graft vs. host reactions, autoimmune diseases (including Raynaud's syndrome, autoimmune thyroiditis, dermatitis, multiple sclerosis, rheumatoid arthritis, insulin-dependent diabetes mellitus, uveitis, inflammatory bowel disease, Crohn's disease, ulcerative colitis or systemic lupus erythematosus), asthma, or the toxic effects of cytokine therapy. Thus, a solution of (R)-3-(3,5-dichlorophenyl)-5-methyl-2-thioxo-5-(4-trifluoromethoxybenzyl)imidazolidin-4-one and aminoacetaldehyde dimethylacetal (6.50 mL, 59.7 mmol) in MeOH was treated with aqueous tert-Bu hydroperoxide solution over 25 min at <20° under ice-cooling, kept at the same

temperature for 1 h , warmed to room temperature, and stirred for 86 h to give (R)-3-(3,5-dichlorophenyl)-2-[(*(E*)-2,2-dimethoxyethyl)imino]-5-methyl-5-(4-trifluoromethoxybenzyl)imidazolidin-4-one which was heated in the presence of p-MeC₆H₄SO₃H in acetone at reflux for 2 h to give (R)-1-(3,5-dichlorophenyl)-3-methyl-3-(4-trifluoromethoxybenzyl)-1H-imidazo[1,2-a]imidazol-2-one.

- IC ICM A61K031-4188
ICS C07D487-04; A61P029-00
CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
IT 2854-16-2P, 2-Hydroxy-2-methylpropyl-1-amine . 86150-21-2P,
(S)-Pyrrolidine-2-carboxylic acid (2-hydroxyethyl)amide 102774-95-8P,
(R)-(-)-Dihydro-5-(azidomethyl)-2(3H)-furanone 137862-22-7P,
(S)-1-(tert-Butoxycarbonyl)pyrrolidine-2-carboxylic acid
(2-hydroxyethyl)amide 321656-41-1P, (S)-1-[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid 321656-51-3P, (S)-1-[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid amide 321657-06-1P,
(R)-3-(4-Cyanobenzyl)-1-(3,5-dichlorophenyl)-3-methylimidazo[1,2-a]imidazol-2-one 321657-07-2P, (R)-5-(4-Bromobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazole-3-sulfonyl chloride 321724-08-7P, (R)-3-(4-Cyanobenzyl)-1-(3,5-dichlorophenyl)-5-iodo-3-methyl-1H-imidazo[1,2-a]imidazol-2-one 688756-08-3P, (R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazole-3-sulfonyl chloride 688756-14-1P, (2R,5R)-2-tert-Butyl-3-(3,5-dichlorophenyl)-5-methyl-1-(2,2,2-trifluoroacetyl)-5-(4-trifluoromethoxybenzyl)imidazolidin-4-one 688756-15-2P, (R)-2-Amino-N-(3,5-dichlorophenyl)-2-methyl-3-(4-trifluoromethoxyphenyl)propionamide 688756-16-3P, (R)-3-(3,5-Dichlorophenyl)-5-methyl-2-thioxo-5-(4-trifluoromethoxybenzyl)imidazolidin-4-one 688756-18-5P, (R)-1-(3,5-Dichlorophenyl)-5-iodo-3-methyl-3-(4-trifluoromethoxybenzyl)-1H-imidazo[1,2-a]imidazol-2-one 689261-01-6P, (R)-3-(3,5-Dichlorophenyl)-2-[(*(E*)-2,2-dimethoxyethyl)imino]-5-methyl-5-(4-trifluoromethoxybenzyl)imidazolidin-4-one 691906-14-6P
691906-17-9P, 1-[(S)-1-[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl)piperidine-4-carboxylic acid methyl ester 691906-26-0P, (S)-Pyrrolidine-2-carboxylic acid N-(2-hydroxy-2-methylpropyl)amide hydrochloride 691906-29-3P
691906-30-6P, (S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid tert-butyl ester 691906-90-8P, (S)-2-[[[(S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]-3-(tert-butoxy)propionic acid tert-butyl ester 691906-93-1P, (S)-1-[(R)-5-(4-Bromobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxy-2-methylpropyl)amide 691906-94-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of [dihydro-5H-imidazo[1,2-a]imidazolylsulfonyl]pyrrolidinecarboxylic acid amide derivs. for treatment of inflammatory diseases)
IT 321656-42-2P, (S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP

(Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of [dihydro-5H-imidazo[1,2-

a]imidazolylsulfonyl]pyrrolidinecarb

oxylic acid amide derivs. for treatment of inflammatory diseases)

IT 688756-17-4P, (R)-1-(3,5-Dichlorophenyl)-3-methyl-3-(4-trifluoromethoxybenzyl)-1H-imidazo[1,2-a]imidazol-2-one
691906-09-9P, (S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-(4-trifluoromethoxybenzyl)-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(2-hydroxy-2-methylpropyl)amide 691906-11-3P, (S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-(4-trifluoromethoxybenzyl)-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(2-hydroxyethyl)amide 691906-12-4P, (S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-(4-trifluoromethoxybenzyl)-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(carbamoylmethyl)amide 691906-13-5P, (R)-2-[(S)-1-[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]propionic acid 691906-15-7P,
[(S)-1-[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]acetic acid 691906-16-8P, 1-[(S)-1-[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]piperidine-4-carboxylic acid 691906-18-0P, (S)-1-[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-((S)-2-hydroxypropyl)amide 691906-19-1P, (S)-1-[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxy-1,1-dimethylethyl)amide 691906-20-4P, (S)-1-[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(furan-2-ylmethyl)amide 691906-21-5P, (S)-1-[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(4-hydroxyphenyl)amide 691906-22-6P, (S)-1-[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(3-hydroxyphenyl)amide 691906-23-7P, (S)-1-[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid acetyl amide 691906-24-8P, (S)-1-[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-[(R)-5-oxotetrahydrofuran-2-yl)methyl]amide 691906-25-9P, (S)-1-[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxy-2-methylpropyl)amide 691906-27-1P 691906-28-2P,
(S)-1-[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxyethyl)amide 691906-31-7P, (S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-methoxyethyl)amide 691906-32-8P,
(S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(2-acetylaminooethyl)amide 691906-33-9P
691906-34-0P 691906-35-1P, (S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-

imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid
 (2-hydroxy-2-methylpropyl)amide **691906-36-2P**,
 (S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-
 yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-
 2-carboxylic acid (2-hydroxyethyl)amide **691906-37-3P**,
 (S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-
 yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-
 2-carboxylic acid [2-(morpholin-4-yl)ethyl]amide **691906-38-4P**
691906-39-5P, [2-[[[(S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-
 oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-
 yl]sulfonyl]pyrrolidine-2-yl]carbonyl]amino]ethyl]carbamic acid tert-butyl
 ester **691906-40-8P**, (S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-
 6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-
 yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-aminoethyl)amide
691906-41-9P, (S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-
 [4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-
 yl]sulfonyl]pyrrolidine-2-carboxylic acid (3-hydroxypropyl)amide
691906-42-0P, (S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-
 [4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-
 yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(furan-2-ylmethyl)amide
691906-43-1P, (S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-
 [4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-
 yl]sulfonyl]pyrrolidine-2-carboxylic acid (2,3-dihydroxypropyl)amide
691906-44-2P, (S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-
 [4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-
 yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxy-1-methylethyl)amide
691906-45-3P, (S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-
 [4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-
 yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(cyanomethyl)amide
691906-46-4P, (S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-
 [4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-
 yl]sulfonyl]pyrrolidine-2-carboxylic acid N-((R)-2-hydroxy-1-
 methylethyl)amide **691906-47-5P**, (S)-1-[[[(R)-7-(3,5-
 Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-
 imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid
 N-((S)-1-hydroxymethyl-3-methylbutyl)amide **691906-48-6P**,
 (S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-
 yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-
 2-carboxylic acid ((R)-1-hydroxymethyl-3-methylbutyl)amide
691906-49-7P, (S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-
 [4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-
 yl]sulfonyl]pyrrolidine-2-carboxylic acid [2-hydroxy-1-
 (hydroxymethyl)ethyl]amide **691906-50-0P**, (S)-1-[[[(R)-7-(3,5-
 Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-
 imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid
 N-(2-aminophenyl)amide **691906-51-1P**, (S)-1-[[[(R)-7-(3,5-
 Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-
 imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid
 N-(3-aminophenyl)amide **691906-52-2P**, (S)-1-[[[(R)-7-(3,5-
 Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-
 imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid
 N-(4-aminophenyl)amide **691906-53-3P**, (S)-1-[[[(R)-7-(3,5-
 Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-
 imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid
 N-(biphenyl-4-yl)amide **691906-54-4P**, (S)-1-[[[(R)-7-(3,5-
 Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-
 imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid
 N-(quinolin-6-yl)amide **691906-55-5P**, (S)-1-[[[(R)-7-(3,5-
 Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-
 imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid

N-[4-(morpholin-4-yl)phenyl]amide **691906-56-6P**,
 (S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(1-methyl-4-oxo-4,5-dihydro-1H-imidazol-2-yl)amide
691906-57-7P, (S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(1,3,5-trimethyl-1H-pyrazol-4-yl)amide **691906-58-8P**, (S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(4-oxo-4,5-dihydrothiazol-2-yl)amide **691906-59-9P**
691906-60-2P, (S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(2-ethyl-2H-pyrazol-3-yl)amide
691906-61-3P, (S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxy-1,1-dimethylethyl)amide **691906-62-4P**, (S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid ((S)-2-hydroxypropyl)amide **691906-63-5P**, (S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid ((R)-2-hydroxypropyl)amide **691906-64-6P**, (R)-1-(3,5-Dichlorophenyl)-5-[(S)-2-[((R)-3-hydroxypyrrolidin-1-yl)carbonyl]pyrrolidin-1-yl]sulfonyl]-3-methyl-3-[4-(pyrimidin-5-yl)benzyl]-1H-imidazo[1,2-a]imidazol-2-one **691906-65-7P**,
 (S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-methyl-N-(carbamoylmethyl)amide **691906-66-8P**,
 (S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid ((S)-1-methylcarbamoylethyl)amide **691906-67-9P**,
 1-[(S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl)piperidine-4-carboxylic acid amide **691906-68-0P**,
 (R)-1-(3,5-Dichlorophenyl)-5-[(S)-2-[(S)-3-hydroxypyrrolidin-1-yl]carbonyl]pyrrolidin-1-yl]sulfonyl]-3-methyl-3-[4-(pyrimidin-5-yl)benzyl]-1H-imidazo[1,2-a]imidazol-2-one **691906-69-1P**,
 1-[(S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino)cyclopropanecarboxylic acid methyl ester
691906-70-4P, (S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(4,5-dihydrooxazol-2-yl)amide
691906-71-5P, (S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(1H-tetrazol-5-ylmethyl)amide
691906-72-6P, (R)-2-[(S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]propionic acid
691906-73-7P, (S)-2-[(S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]propionic acid
691906-74-8P, [(S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]acetic acid
691906-75-9P, [N-[(S)-1-[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]N-methylamino]acetic acid

691906-76-0P, 2-[[[(S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]-2-methylpropionic acid
691906-77-1P, 3-[[[(S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]propionic acid
691906-78-2P, 1-[[[(S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]piperidine-4-carboxylic acid
691906-79-3P, 6,7-Dihydro-3-[[[(S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]-4,4,4-trifluorobutyric acid methyl ester **691906-80-6P**, 3-[[[(S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]-4,4,4-trifluorobutyric acid ethyl ester
691906-81-7P, (S)-2-[[[(S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl](methyl)amino]-3-methylbutyric acid
691906-82-8P, (1S,2S)-2-[[[(S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]cyclohexanecarboxylic acid **691906-83-9P**, 3-[[[(S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]butyric acid
691906-84-0P, 3-[[[(S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]-2-methylpropionic acid
691906-85-1P, 1-[[[(S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]cyclopropanecarboxylic acid
691906-86-2P, (S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-carbamoylethyl)amide
691906-87-3P, (S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid ((R)-1-carbamoylethyl)amide
691906-88-4P, (S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (1-carbamoyl-1-methylethyl)amide
691906-89-5P, (S)-2-[[[(S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]-3-hydroxypropionic acid
691906-91-9P, (S)-1-[[[(R)-5-[4-(4-Aminopyrimidin-5-yl)benzyl]-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxy-2-methylpropyl)amide **691906-95-3P**, (S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(2-fluoropyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxy-2-methylpropyl)amide **691906-96-4P**, (S)-1-[[[(R)-5-[4-(4-Aminopyrimidin-5-yl)benzyl]-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxyethyl)amide
691906-97-5P, (S)-1-[[[(R)-7-(3,5-Dichlorophenyl)-5-[4-(2-fluoropyrimidin-5-yl)benzyl]-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxyethyl)amide **691906-98-6P**, (S)-1-[[[(R)-5-[4-(2-Cyanopyridin-3-yl)benzyl]-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxy-2-methylpropyl)amide **691906-99-7P**,

(S)-1-[(*R*)-5-[4-(2-Cyanopyridin-3-yl)benzyl]-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5*H*-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(carbamoylmethyl)amide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of [dihydro-5*H*-imidazo[1,2-

a]imidazolylsulfonyl]pyrrolidinecarb
oxylic acid amide derivs. for treatment of inflammatory diseases)
IT 688756-19-6P, (*R*)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-(4-trifluoromethoxybenzyl)-6,7-dihydro-5*H*-imidazo[1,2-a]imidazole-3-sulfonyl chloride

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of [dihydro-5*H*-imidazo[1,2-

a]imidazolylsulfonyl]pyrrolidinecarb
oxylic acid amide derivs. for treatment of inflammatory diseases)

IT 75-86-5, Acetone cyanohydrin 98-74-8, 4-Nitrobenzenesulfonyl chloride 108-24-7, Acetic anhydride 109-85-3, 2-Methoxyethylamine 141-43-5, Ethanolamine, reactions 1668-10-6, Glycinamide hydrochloride 2799-17-9, (*S*)-1-Aminopropan-2-ol 2812-46-6 2971-79-1, Methyl isonipecotate 3196-73-4, β -Alanine methyl ester hydrochloride 15761-39-4 22483-09-6, Aminoacetaldehyde dimethylacetal 32916-51-1, Cyclopentylmagnesium chloride 33240-34-5, Cyclopentylmagnesium bromide 42429-27-6 48067-24-9, O-tert-Butyl-L-serine tert-butyl ester 50824-05-0, 4-Trifluoromethoxybenzyl bromide 52813-63-5, (*R*)-(-)-Dihydro-5-(hydroxymethyl)-2(3*H*)-furanone 53742-62-4, N-(tert-Butyldimethylsilyl)aniline 59531-86-1, D-Alanine tert-butyl ester hydrochloride 59624-87-2 73183-34-3 321656-72-8, (*R*)-3-(4-Bromobenzyl)-1-(3,5-dichlorophenyl)-3-methylimidazo[1,2-a]imidazol-2-one 321656-73-9, (*R*)-3-(4-Bromobenzyl)-1-(3,5-dichlorophenyl)-5-iodo-3-methyl-1*H*-imidazo[1,2-a]imidazol-2-one 321724-17-8, (2*S*,5*R*)-2-tert-Butyl-3-(3,5-dichlorophenyl)-5-methyl-1-(2,2,2-trifluoroacetyl)imidazolidin-4-one 321724-19-0, 5-(4,4,5,5-Tetramethyl-[1,3,2]dioxaborolan-2-yl)pyrimidine 343926-69-2, 2-Amino-4-bromopyrimidine 691906-10-2, (*S*)-2-(2-Hydroxy-2-methylpropylcarbamoyl)pyrrolidine-1-carboxylic acid tert-butyl ester 691906-92-0, L-Pyrrolidine-2-carboxylic acid (2-hydroxy-2-methylpropyl)amide

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant; preparation of [dihydro-5*H*-imidazo[1,2-

a]imidazolylsulfonyl]pyrrolidinecarboxylic acid amide derivs. for treatment of inflammatory diseases)

L23 ANSWER 10 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:991342 ZCPLUS Full-text

DOCUMENT NUMBER: 140:42161

TITLE: Preparation of substituted 3-amino-thieno[2,3-b]pyridine-2-carboxylic acid amide compounds and processes for preparing and their uses as inhibitors of IKB kinase complex

INVENTOR(S): Cywin, Charles L.; Chen, Zhidong; Emeigh, Jonathan; Fleck, Roman Wolfgang; Hao, Ming-hong; Hickey, Eugene; Liu, Weimin; Marshall, Daniel Richard; Morwick, Tina; Nemoto, Peter; Sorcek, Ronald John; Sun, Sanxing; Wu, Jiang-ping

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 165 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

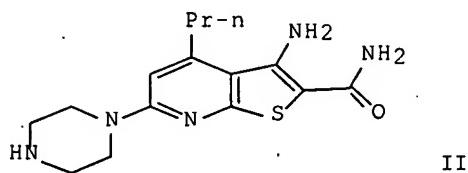
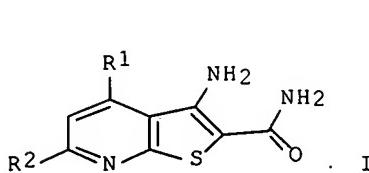
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003103661	A1	20031218	WO 2003-US17343	20030603
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2483890	A1	20031218	CA 2003-2483890	20030603
AU 2003237330	A1	20031222	AU 2003-237330	20030603
US 2004053957	A1	20040318	US 2003-453175	20030603
US 6964956	B2	20051115		
BR 2003011605	A	20050222	BR 2003-11605	20030603
EP 1513516	A1	20050316	EP 2003-736796	20030603
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1649581	A	20050803	CN 2003-809958	20030603
JP 2005530816	T	20051013	JP 2004-510780	20030603
NZ 537394	A	20061222	NZ 2003-537394	20030603
US 2004180922	A1	20040916	US 2003-730172	20031206
US 6974870	B2	20051213		
IN 2004DN03224	A	20050401	IN 2004-DN3224	20041019
NO 2004004599	A	20050216	NO 2004-4599	20041025
US 2005288285	A1	20051229	US 2005-206707	20050818
RITY APPLN. INFO.:			US 2002-386312P	P 20020606
			US 2003-457867P	P 20030326
			US 2003-453175	A1 20030603
			WO 2003-US17343	W 20030603

OTHER SOURCE(S) : MARPAT 140:42161

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AB Title compds. I [R1 = (un)substituted-Ph, -heteroaryl, -heterocyclyl, -alkyl, -alkoxy, etc.; R2 = (un)substituted-alkyl, -alkoxy, -alkylamino, -alkylthio, -Ph, -heterocyclyl, etc.], and their pharmaceutically acceptable salts, are prepared and disclosed as inhibitors of the kinase activity of the IKK kinase (IKK) complex. Thus, e.g., II was prepared in five steps by cyclization of Me 2-hexynoate with 2-cyanothioacetamide in the presence of morpholine to provide intermediate mercaptopyridone which is S-alkylated with 2-bromoacetamide,

converted to the O-triflate derivative, reacted with 1-BOC-piperazine and deprotected. I possessed IC50's of 10 μ M or below in assays for inhibition of IKK β . The compds. are therefore useful in the treatment of IKK mediated diseases including autoimmune diseases, inflammatory diseases and cancer. Also disclosed are pharmaceutical compns. comprising these compds. and processes for preparing these compds.

IC ICM A61K031-38
ACCESSION NUMBER: 2002:487567 ZCPLUS Full-text

CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 11 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:487567 ZCPLUS Full-text
DOCUMENT NUMBER: 137:52411
TITLE: Small molecules useful in the treatment of inflammatory disease
INVENTOR(S): Fleck, Roman Wolfgang; Kelly, Terence Alfred ; Kim, Jin Mi; Lee, Jinbo; Lemieux, Rene Marc ; Sorcek, Ronald John; Wu, Jiang-Ping
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 75 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002050080	A1	20020627	WO 2001-US46649	20011205
W: CA, JP, MX RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
US 2003008848	A1	20030109	US 2001-11070	20011205
			US 2000-256811P	P 20001219

PRIORITY APPLN. INFO.: MARPAT 137:52411

OTHER SOURCE(S): AB A method for treating or preventing inflammatory and immune cell-mediated diseases by the administration of certain small heterocyclic compds. are described. These compds. act by inhibiting interaction of cellular adhesion mols. (including ICAM-1, ICAM-2, and ICAM-3) with the leukointegrins (especially CD18/CD11a). Pharmaceutical compns. comprising these small heterocyclic compds., such as capsules, tablets, parenteral solns., suspensions or topical formulations, suitable for the prevention or treatment of inflammatory and immune cell-mediated diseases are also described.

IC ICM C07D487-04
ACCESSION NUMBER: 2002:182177 ZCPLUS Full-text

CC 63-6 (Pharmaceuticals)

Section cross-reference(s): 1, 28

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

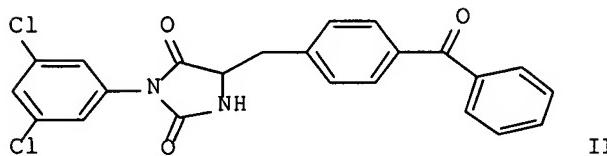
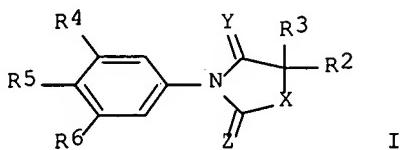
L23 ANSWER 12 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:182177 ZCPLUS Full-text
DOCUMENT NUMBER: 136:232302
TITLE: Preparation of 1-phenyl-2,5-imidazolidinediones and analogs for treatment of inflammatory and immune cell-mediated diseases

INVENTOR(S): *Kelly, Terence A.; Bormann, Barbara Jean;
 Frye, Leah Lynn; Wu, Jiang-Ping*
 PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
 SOURCE: U.S., 114 pp., Cont.-in-part of Appl. No.
 PCT/US98/04254.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6355664	B1	20020312	US 1999-375010	19990816
WO 9839303	A1	19980911	WO 1998-US4254	19980303
		W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG		
US 38132	E1	20030603	US 2002-167732	20020612
PRIORITY APPLN. INFO.:			US 1997-40011P	P 19970303
			US 1998-33148	B2 19980302
			WO 1998-US4254	A2 19980303
			US 1999-375010	A5 19990816

OTHER SOURCE(S): MARPAT 136:232302

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AB Title imidazolidinediones, pyrrolidinediones, oxazolidinediones, and thiazolidinediones I [wherein Y = O or S; Z = O or S; X = CHR1, NR1, CHSO2R1, or NSO2R1; R1 = H, carboxylic acid group, phosphonic acid group, sulfonic acid group, imidamidoalkyl, guanidinoalkyl, or (un)substituted (cyclo)alkyl, piperidyl, or aryl; R2 = H or (un)substituted (cyclo)alkyl; R3 = H or (un)substituted aryl(alkyl); R4 = Cl or CF3; R5 and R6 = independently H, halo, Me, or CF3; and pharmaceutically acceptable salts] were prepared as intracellular adhesion mols. (ICAMs) and leukointegrin antagonists. For example, reaction of 4-benzoyl-DL-phenylalanine with 3,5-

dichlorophenylisocyanate and cyclization of the ureidoacetic acid intermediate gave II. The latter inhibited lymphocyte function-associated 1 (LFA-1) binding to ICAM-1 with K_d of 1.64 μM . I are useful for the treatment of inflammatory and immune cell-mediated disorders, such as psoriasis, organ/tissue transplant rejection, graft vs. host reactions, autoimmune diseases, asthma, and toxicity associated with cytokine therapy.

IC ICM A61K031-4439
ICS A61K031-4166; C07D401-10; C07D233-40

INCL 514389000

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 34

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 13 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:202160 ZCPLUS Full-text

TITLE: Small molecule antagonists of LFA-1 mediated cell adhesion

AUTHOR(S): *Emeigh, Jonathan E.; Bormann, Barbara-Jean; Frye, Leah L.; Jeanfavre, Deborah D.; McNeil, Daniel W.; Nabozny, Gerald H.; Stefany, David W.; Woska, Joseph R., Jr.; Wu, Jiang-Ping; Zindell, Renee; Zinter, Rosemary; Kelly, Terence A.*

CORPORATE SOURCE: Medicinal Chemistry Department, Boehringer Ingelheim Pharmaceuticals, Inc, Ridgefield, CT, 06810, USA

SOURCE: Abstracts of Papers, 221st ACS National Meeting, San Diego, CA, United States, April 1-5, 2001 (2001)
MEDI-256

CODEN: 69FZD4

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal; Meeting Abstract

LANGUAGE: English

AB Lymphocyte function-associated antigen 1 (LFA-1) is a cellular adhesion mol. involved in many fundamental immunol. processes such as leukocyte trafficking, antigen presentation, B-cell activation, and activation of cytotoxic T lymphocytes. Modulation of these LFA-1 mediated events may lead to useful therapeutic agents for autoimmune disorders. In this poster, we report on the structure-activity relationships of a novel class of small mols. (e.g. BIRT0377) that blocks the interactions between LFA-1 and one of its adhesion partners, ICAM-1.

L23 ANSWER 14 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:78387 ZCPLUS Full-text

DOCUMENT NUMBER: 134:131538

TITLE: Preparation of imidazoimidazoles and triazoles as anti-inflammatory agents

INVENTOR(S): *Wu, Jiang-Ping; Kelly, Terence Alfred; Lemieux, Rene M.; Goldberg, Daniel R.; Emeigh, Jonathan Emilian; Sorcek, Ronald J.*

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 368 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.

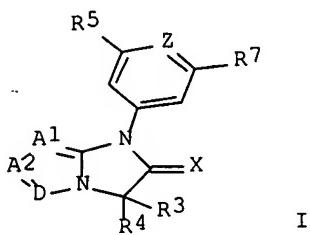
KIND DATE

APPLICATION NO.

DATE

WO 2001007440	A1	20010201	WO 2000-US18884	20000712
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6492408	B1	20021210	US 2000-604312	20000627
CA 2383017	A1	20010201	CA 2000-2383017	20000712
BR 2000012666	A	20020409	BR 2000-12666	20000712
EP 1216247	A1	20020626	EP 2000-948618	20000712
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
TR 200200160	T2	20021021	TR 2002-160	20000712
JP 2003505460	T	20030212	JP 2001-512524	20000712
HU 200203971	A2	20030328	HU 2002-3971	20000712
EE 200200028	A	20030415	EE 2002-28	20000712
NZ 517217	A	20040227	NZ 2000-517217	20000712
AU 776496	B2	20040909	AU 2000-62091	20000712
TW 261591	B	20060911	TW 2000-89114536	20000720
IN 2002MN00002	A	20060915	IN 2002-MN2	20020102
BG 106312	A	20020930	BG 2002-106312	20020116
ZA 2002000428	A	20030117	ZA 2002-428	20020117
NO 2002000275	A	20020204	NO 2002-275	20020118
NO 322707	B1	20061127		
US 2003203955	A1	20031030	US 2002-195973	20020716
US 6689804	B2	20040210		
HK 1048637	A1	20050225	HK 2003-100839	20030206
US 2004116426	A1	20040617	US 2003-672412	20030925
PRIORITY APPLN. INFO.:			US 1999-144905P	P 19990721
			US 1999-150939P	P 19990826
			US 2000-604312	A1 20000627
			WO 2000-US18884	W 20000712
			US 2002-195973	A3 20020716

OTHER SOURCE(S): MARPAT 134:131538
GI



AB Compds. I {A1 = N, CH; A2 = N, CH, CR'; R' = halo, cyano, alkoxy, alkoxycarbonyl, alkylsulfonyl; D = N, CH, CR1, C(S(:O)R1), C[S(:O)R1], C(CHO),

C(SR₁a), C(OR₁a), C(NHR₁a); R₁, R₁a = (substituted) alkyl, cycloalkyl, aryl, or heteroaryl groups, alkyl groups containing 2-6 carbons substituted with carboxylate, phosphonate, sulfonate, amidine, or guanidine moieties, amino, halogen, cyano; R₃ = H, alkyl, cycloalkyl, alkoxy or amino substituted alkyl, cycloalkyl; R₄ = substituted arylmethyl; R₅ = Cl, F3C; R₇ = H, halo, Me, cyano, O2N, F3C; X = O, S; if Z = N or CH, R₇ = Cl, F3C, cyano, O2N; Z = N, CR₆ where R₆ = H, halo, Me, cyano, F3C}, based mostly on imidazo[1,2-a]imidazole and imidazo[1,2-a]triazole nuclei, are prepared as inhibitors of the binding of leukointegrins to cell adhesion mols. in the treatment or prevention of inflammatory and immune cell-mediated diseases. E.g., (R)-I (A₁ = N; A₂ = D = CH; R₃ = Me; R₄ = 4-BrC₆H₄CH₂; R₅ = R₇ = Cl; X = O; Z = CH) (II) was prepared from (R)- α -methyl-4-bromophenylalanine Me ester and 3,5-dichlorophenylisothiocyanate by heating in 1,4-dioxane to give a thiohydrantoin which was treated with N-(triphenylphosphoranylidene)-1,3-dioxolan-2-ylmethylamine [prepared from 2-(azidomethyl)-1,3-dioxolane and triphenylphosphine] to give a dioxolanylmethylinimidoimidolidinone derivative; treatment of the intermediate with trifluoroacetic acid and heating at 90° overnight gave II with m.p. 36-37.5°. I inhibited binding of leukointegrins to cell adhesion mols. with Kd<10 μ M.

IC	ICM C07D487-04
	ICS C07F009-40; C07D519-00; C07F009-38; A61K031-41; A61K031-415; A61P029-00; C07D487-04; C07D233-00; C07D487-04; C07D233-00; C07D249-00; C07D487-04; C07D233-00; C07D257-00
CC	28-9 (Heterocyclic Compounds (More Than One Hetero Atom)) Section cross-reference(s): 1
IT	321656-35-3P 321656-59-1P 321656-61-5P 321656-64-8P 321656-68-2P 321656-72-8P 321656-73-9P 321656-74-0P 321656-99-9P 321657-06-1P 321657-07-2P 321657-64-1P 321724-09-8P
	RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of imidazoimidazole and imidazotriazole derivs. as inhibitors of leukointegrin binding to cell adhesion mols. in the treatment of inflammatory and immune-cell mediated diseases)
IT	321656-36-4P 321656-37-5P 321656-38-6P 321656-39-7P 321656-41-1P 321656-42-2P 321656-43-3P 321656-51-3P 321656-52-4P 321656-53-5P 321656-54-6P 321656-57-9P 321656-58-0P 321656-60-4P 321656-62-6P 321656-63-7P 321656-65-9P 321656-66-0P 321656-67-1P 321656-69-3P 321656-70-6P 321656-71-7P 321656-81-9P 321656-89-7P 321656-95-5P 321657-00-5P 321657-01-6P 321657-02-7P 321657-03-8P 321657-04-9P 321657-05-0P 321657-08-3P 321657-25-4P 321657-77-6P 321657-89-0P 321657-90-3P 321657-91-4P 321718-69-8P 321718-71-2P 321718-73-4P 321718-75-6P 321718-77-8P 321718-79-0P 321718-81-4P 321718-83-6P 321718-85-8P 321718-87-0P 321718-89-2P 321718-91-6P 321718-93-8P 321718-95-0P 321718-97-2P 321718-99-4P 321719-01-1P 321719-03-3P 321719-05-5P 321719-07-7P 321719-09-9P 321719-11-3P 321719-13-5P 321719-15-7P 321719-17-9P 321719-19-1P 321719-21-5P 321719-23-7P 321719-25-9P 321719-27-1P 321719-29-3P 321719-31-7P

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321719-69-1P 321719-71-5P 321719-73-7P
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321719-82-8P 321719-84-0P 321719-86-2P
321719-88-4P 321719-90-8P 321719-92-0P
321719-94-2P 321719-96-4P 321719-98-6P
321720-00-7P 321720-02-9P 321720-04-1P
321720-06-3P 321720-08-5P 321720-10-9P
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321722-92-3P 321722-93-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of imidazoimidazole and imidazotriazole derivs. as inhibitors of leukointegrin binding to cell adhesion mols. in the treatment of

inflammatory and immune-cell mediated diseases)

IT 321722-94-5P 321722-95-6P 321722-96-7P
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 321724-03-2P 321746-08-1P 321746-09-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of imidazoimidazole and imidazotriazole derivs. as inhibitors of leukointegrin binding to cell adhesion mols. in the treatment of inflammatory and immune-cell mediated diseases)

IT 321724-20-3P

RL: BYP (Byproduct); PREP (Preparation)

(preparation of imidazoimidazole and imidazotriazole derivs. as inhibitors of leukointegrin binding to cell adhesion mols. in the treatment of inflammatory and immune-cell mediated diseases)

IT 110-85-0, Piperazine, reactions 874-24-8, 3-Hydroxypicolinic acid 1692-25-7, 3-Pyridineboronic acid 2133-40-6, L-Proline methyl ester hydrochloride 3235-69-6, 4-Morpholineacetic acid 6165-69-1, 3-Thiopheneboronic acid 13889-98-0, N-Acetylpirperazine 17201-43-3, α -Bromo-p-tolunitrile 50585-89-2, Methyl nipecotate 57260-71-6 69849-42-9, 5-(Trimethylstannyl)pyrimidine 131534-65-1 156545-07-2, 3,5-Difluorophenylboronic acid 321724-14-5 321724-15-6 321724-16-7 321724-17-8 321724-18-9 321724-19-0 321724-21-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of imidazoimidazole and imidazotriazole derivs. as inhibitors of leukointegrin binding to cell adhesion mols. in the treatment of

inflammatory and immune-cell mediated diseases)

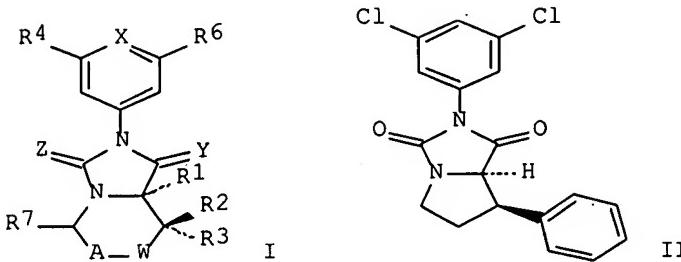
IT 321724-04-3P 321724-05-4P 321724-06-5P 321724-07-6P
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321724-13-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of imidazoimidazole and imidazotriazole derivs. as inhibitors of leukointegrin binding to cell adhesion mols. in the treatment of inflammatory and immune-cell mediated diseases)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 15 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:78243 ZCPLUS Full-text
DOCUMENT NUMBER: 134:131537
TITLE: Novel N-aryl cycloalkyl fused imidazolediones useful in the treatment of inflammatory disease
INVENTOR(S): Kelly, Terence Alfred; Wu, Jiang-Ping; Kuzmich, Daniel
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 114 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001007052	A1	20010201	WO 2000-US17752	20000628
W: CA, JP, MX RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 6365615	B1	20020402	US 2000-605675 US 1999-144894P	20000628 P 19990721
PRIORITY APPLN. INFO.:				
OTHER SOURCE(S): GI	MARPAT	134:131537		



AB Novel N-aryl cycloalkyl fused imidazolediones I [Y and Z independently = O or S; R1 = H, (un)substituted unbranched or branched alkyl or cycloalkyl, alkoxy or acyloxy; R2 = (un)substituted aryl; R3 = H, OH, alkoxy, acyloxy, or (un)substituted unbranched or branched alkyl or cycloalkyl; R4 = Cl or CF₃; X

= N or CR₅ where R₅ = H, halo, Me, or CF₃; R₆ = H, halo, Me, CN, NO₂ or CF₃ with condition that when X = N or CH, R₆ = Cl or CF₃; A = (CHR₈)_m where m = 0 or 1; W = (CHR₉)_n where n = 0 or 1 and m + n = 1 or 2; R₇, R₈ and R₉ independently = H, oxo, R₁₀, OR₁₀, NHR₁₀, COR₁₀, CONHR₁₀, CO₂R₁₀, SO₂R₁₀ or SR₁₀ wherein R₁₀ = H, (un)substituted branched or unbranched alkyl or cycloalkyl, alkylcarboxylic acid, alkylphosphonic acid, alkylamidino, etc.] which are useful for treating or preventing inflammatory and immune cell-mediated diseases are disclosed as well as methods for their preparation. Thus, II was prepared in four steps via a cyclocondensation reaction of an intermediate N-(3,5-dichlorophenylamido)-3-phenylpyrrolidin-2-yl carboxylic acid. The title compds. possessed Kd values < 10 μM for inhibition of LFA-1 binding to ICAM-1. Pharmaceutical compns. of I suitable for prevention or treatment of inflammatory and immune cell-mediated conditions are disclosed.

IC ICM A61K031-55

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 63

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 16 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:78239 ZCPLUS Full-text

DOCUMENT NUMBER: 134:131536

TITLE: Novel N-(pyridin-4-yl) nitrogen heterocyclic compounds useful in the treatment of inflammatory disease

INVENTOR(S): Kelly, Terence Alfred; Sorcek, Ronald John

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 101 pp.

CODEN: PIXXD2

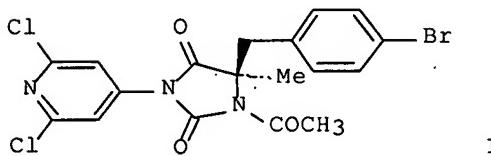
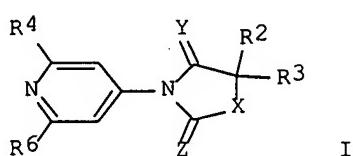
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001007048	A1	20010201	WO 2000-US17806	20000628
W: CA, JP, MX RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 6350763	B1	20020226	US 2000-604899 US 1999-144844P	20000628 P 19990721
PRIORITY APPLN. INFO.:				
OTHER SOURCE(S): MARPAT 134:131536				
GI				



AB Novel N-(pyridin-4-yl) nitrogen heterocyclic compds. I [Y and Z are independently O or S; X = O, S, CHR1, NR1, CHSO2R1 or NSO2R1; R1 = H, (un)substituted branched or unbranched alkyl, alkylcarboxylic acid, alkylphosphonic acid, alkylamidino, N-substituted piperidyl, etc.; R2 = H, (un)substituted branched or unbranched alkyl or cycloalkyl; R3 = (CR7R8)x(CR9R10)yR11 where x and y independently = 0 or 1; R7, R8, and R9 independently = H, OH, alkoxy, acyloxy, branched or unbranched alkyl or cycloalkyl; R10 = H, OH, alkoxy, acyloxy, branched or unbranched alkyl or cycloalkyl, (un)substituted aryl; R11 = (un)substituted aryl; R4 = Cl, CF3; R6 = halo, Me, CF3, CN or NO2] which are useful for treating or preventing inflammatory and immune cell-mediated diseases (no data) are disclosed as well as methods for their preparation Thus, II was prepared by cyclocondensation of 4-amino-2,6-dichloropyridine with (R)- α -methyl-4-bromophenylalanine Me ester isocyanate and quenched with acetic anhydride. Pharmaceutical compns. of I suitable for prevention or treatment of inflammatory and immune cell-mediated conditions are disclosed.

IC ICM A61K031-44

ICS A61K031-675; C07F009-06; C07D401-00; C07D401-04; C07D401-14; C07D413-00; C07D417-04; C07D417-14

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 63

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 17 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:78235 ZCPLUS Full-text

DOCUMENT NUMBER: 134:131534

TITLE: Novel N-aryl nitrogen heterocyclic compounds useful in the treatment of inflammatory disease

INVENTOR(S): Kelly, Terence Alfred; Sorcek, Ronald John

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 101 pp.

CODEN: PIXXD2

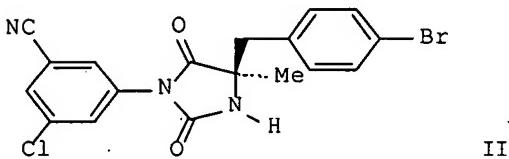
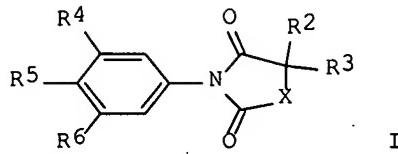
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001007044	A1	20010201	WO 2000-US17712	20000628
W: CA, JP, MX				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 6353013	B1	20020305	US 2000-605574	20000628
PRIORITY APPLN. INFO.:			US 1999-144893P	P 19990721
OTHER SOURCE(S):	MARPAT	134:131534		
GI				



AB Novel N-aryl nitrogen heterocyclic compds. I [Y and Z are independently O or S; X = O, S, CHR1, NR1, CHSO2R1 or NSO2R1; R1 = H, (un)substituted branched or unbranched alkyl, alkylcarboxylic acid, alkylphosphonic acid, alkylamidino, N-substituted piperidyl, etc.; R2 = H, (un)substituted branched or unbranched alkyl or cycloalkyl; R3 = (CR7R8)x(CR9R10)yR11 where x and y independently = 0 or 1; R7, R8, and R9 independently = H, OH, alkoxy, acyloxy, branched or unbranched alkyl or cycloalkyl; R10 = H, OH, alkoxy, acyloxy, branched or unbranched alkyl or cycloalkyl, (un)substituted aryl; R11 = (un)substituted aryl; R4 = Cl, CF3; R5 = H, halo, Me, CF3; R6 = CN or NO2] which are useful for treating or preventing inflammatory and immune cell-mediated diseases (no data) are disclosed as well as methods for their preparation. Thus, II was prepared by hydrolysis of 5-(R)-(4-bromobenzyl)-3-(5-acetamino-3-chlorophenyl)-5-methylimidazoline-2,4-dione followed by Sandmeyer reaction with NaNO2, CuCN and KCN. Pharmaceutical compns. of I suitable for prevention or treatment of inflammatory and immune cell-mediated conditions are disclosed.

IC ICM A61K031-4164

ICS A61K031-4166; C07D233-76; C07D233-84; C07D233-86

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 18 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:78178 ZCPLUS Full-text

DOCUMENT NUMBER: 134:131424

TITLE: Novel indolones and pyrrolopyridinones useful in the treatment of inflammatory disease

INVENTOR(S): Kelly, Terence Alfred; Wu, Jiang-Ping; Kuzmich, Daniel; Ward, Yancey David; Frye, Leah Lynn

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 100 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

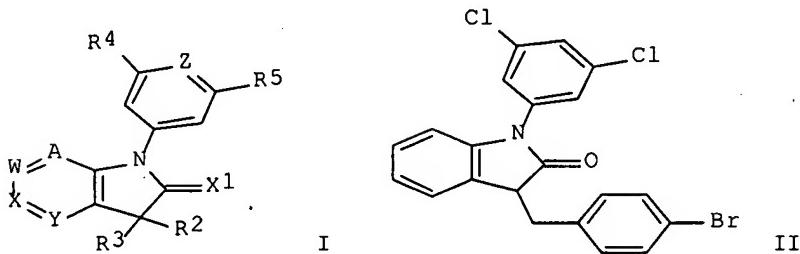
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2001006984	A2 20010201	WO 2000-US17802	20000628
WO 2001006984	A3 20031231		
W: CA, JP, MX			
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE			
CA 2378369	A1 20010201	CA 2000-2378369	20000628
US 6414153	B1 20020702	US 2000-605584	20000628
JP 2004505005	T 20040219	JP 2001-511876	20000628
JP 3833532	B2 20061011		
EP 1399155	A2 20040324	EP 2000-950262	20000628
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY			

PRIORITY APPLN. INFO.: US 1999-144895P P 19990721
WO 2000-US17802 W 20000628

OTHER SOURCE(S): MARPAT 134:131424

GI



AB The title compds. I [A, W, and X independently = N or CH; Y = N, CR1, CSO2R1, CSOR1, CSR1, COR1, CCOR1, CNHRI where R1 = H, (un)substituted branched or unbranched alkyl or cycloalkyl, alkylcarboxylic acid, alkylphosphonic acid, alkylaminodino, etc.; X1 = O, S; R2 = H, (un)substituted branched or unbranched alkyl or cycloalkyl; R3 = (CR6R7)m(CR8R9)nR10 wherein m and n = 0 or 1; R6, R7 and R8 independently = H, OH, alkoxy, acyloxy or (un)substituted branched or unbranched alkyl or cycloalkyl; R9 = R1 or OR1; R10 = (un)substituted aryl; Z = N or CR11 wherein R11 = H, halo, Me or CF3; R4 = Cl or CF3; R5 = H, halo, Me, CN, NO2, CF3 with provision when Z = N or CH, R5 = Cl or CF3] which are useful for treating or preventing inflammatory and immune cell-mediated diseases are disclosed as well as methods for their preparation. Thus, II was prepared via Ullman coupling of indole and 1-bromo-3,5-dichlorobenzene, chlorination and hydrolysis to the indolone intermediate, condensation with 4-bromobenzaldehyde and subsequent hydrogenation. II possessed a Kd value > 10 for inhibition of LFA-1 binding to ICAM-1. Pharmaceutical compns. of I suitable for prevention or treatment of inflammatory and immune cell-mediated conditions are disclosed.

IC ICM A61K

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1, 63

L23 ANSWER 19 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:332327 ZCPLUS Full-text

TITLE: Direct transformation of functionalized aromatic/heteroaromatic halides into sulfones.

AUTHOR(S): Wu, Jiang-Ping; Emeigh, Jonathan

CORPORATE SOURCE: Department of Medicinal Chemistry, Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT, 06877, USA

SOURCE: Book of Abstracts, 219th ACS National Meeting, San Francisco, CA, March 26-30, 2000 (2000), ORGN-201.
American Chemical Society: Washington, D. C.
CODEN: 69CLAC

DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English

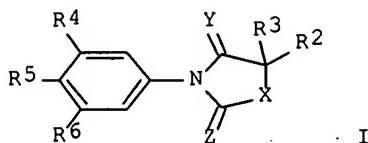
AB A direct transformation of functionalized aromatic/hetero-aromatic halides into sulfones is described. This transformation is a three step-one pot procedure which involves 1) generating Grignard reagents from the aromatic/hetero-aromatic halides by magnesium halides exchange; 2) quenching the Grignard reagents with SO₂ to produce magnesium sulfinate; 3) alkylating the sulfinate intermediates with alkyl bromides or Michael acceptors. This method avoids oxidation reaction necessary in the conventional sulfone preparation through the oxidation of sulfides and is therefore particularly valuable in the preparation of sulfones where the substrates contain oxidizable groups. In addition a variety of functional groups on the substrates are tolerated.

L23 ANSWER 20 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:612077 ZCPLUS Full-text
DOCUMENT NUMBER: 129:260456
TITLE: Small molecules useful in the treatment of inflammatory disease
INVENTOR(S): Kelly, Terence Alfred; Bormann, Barbara Jean; Frye, Leah Lynn; Wu, Jiang-ping
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 361 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9839303	A1	19980911	WO 1998-US4254	19980303
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2278547	A1	19980911	CA 1998-2278547	19980303
AU 9865418	A	19980922	AU 1998-65418	19980303
EP 966447	A1	19991229	EP 1998-911475	19980303
EP 966447	B1	20030305		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
EE 9900481	A	20000615	EE 1999-481	19980303
TR 9902124	T2	20000621	TR 1999-2124	19980303
BR 9811260	A	20000808	BR 1998-11260	19980303
HU 200002347	A2	2001028	HU 2000-2347	19980303
JP 2001513821	T	20010904	JP 1998-538772	19980303
AT 233738	T	20030315	AT 1998-911475	19980303
ES 2191286	T3	20030901	ES 1998-911475	19980303
ZA 9807065	A	20000207	ZA 1998-7065	19980806
US 6355664	B1	20020312	US 1999-375010	19990816

MX 9907583	A 20000228	MX 1999-7583	19990817
NO 9904256	A 19991102	NO 1999-4256	19990902
BG 103711	A 20010928	BG 1999-103711	19990902
US 38132	E1 20030603	US 2002-167732	20020612
PRIORITY APPLN. INFO.:		US 1997-40011P	P 19970303
		US 1998-33148	B2 19980302
		WO 1998-US4254	W 19980303
		US 1999-375010	A5 19990816

OTHER SOURCE(S): MARPAT 129:260456
GI



AB Title small mols. [I; Y = O, S; Z = O, S; X = CH₂, NH, CHSO₂H, etc.; R₂ = H, cycloalkyl, OH, etc.; R₃ = H, OH, alkyloxy, alkyl; R₄ = Cl, CF₃; R₅ = H, F, Cl, Br, I, CH₃, CF₃; R₆ = H, F, Cl, Br, I, CH₃, CF₃] and pharmaceutically acceptable salts are prepared A method treating or preventing inflammatory and immune cell-mediated diseases by the administration of certain novel and known small mols. such as (R)-I (X = NH; Y = O; Z = O; R₂ = CH₃; R₃ = 4-BrC₆H₄CH₂; R₄ = R₆ = Cl; R₅ = H).

IC ICM C07D233-76
ICS C07D233-78; C07D233-74; C07D233-80; A61K031-415; C07D207-40; C07F009-6506; C07F009-6558; C07D401-10; C07D403-06; C07D409-06; C07D401-04; C07D263-44; C07D233-86; A61K031-675

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 34, 63

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 21 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:187082 ZCPLUS Full-text
DOCUMENT NUMBER: 126:233098
TITLE: Effect of Structural Modification of Enol-Carboxamide-Type Nonsteroidal Antiinflammatory Drugs on COX-2/COX-1 Selectivity
AUTHOR(S): Lazer, Edward S.; Miao, Clara K.; Cywin, Charles L.; Sorcek, Ronald; Wong, Hin-Chor; Meng, Zhaoxing; Potocki, Ian; Hoermann, MaryAnn; Snow, Roger J.; Tschantz, Matt A.; Kelly, Terence A.; McNeil, Daniel W.; Coutts, Simon J.; Churchill, Laurie; Graham, Anne G.; David, Eva; Grob, Peter M.; Engel, Wolfhard; Meier, Hans; Trummlitz, Guenter
CORPORATE SOURCE: Department of Inflammatory Diseases, Boehringer Ingelheim Pharmaceuticals Inc., Ridgefield, CT, 06877, USA
SOURCE: Journal of Medicinal Chemistry (1997), 40(6), 980-989
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Meloxicam, an NSAID in the enol-carboxamide class, was developed on the basis of its antiinflammatory activity and relative safety in animal models. In subsequent screening in microsomal assays using human COX-1 and COX-2, we discovered that it possessed a selectivity profile for COX-2 superior to piroxicam and other marketed NSAIDs. We therefore embarked on a study of enol-carboxamide type compds. to determine if COX-2 selectivity and potency could be dramatically improved by structural modification. Substitution at the 6- and 7-positions of the 4-oxo-1,2-benzothiazine-3- carboxamide, alteration of the N-Me substituent, and amide modification were all examined. In addition we explored several related systems including the isomeric 3-oxo-1,2-benzothiazine-4-carboxamides, thienothiazines, indolothiazines, benzothienothiazines, naphthothiazines, and 1,3- and 1,4-dioxoisouquinolines. While a few examples were found with greater potency in the COX-2 assay, no compound tested had a better COX-2/COX-1 selectivity profile than that of meloxicam.

CC 1-3 (Pharmacology)

Section cross-reference(s): 28

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 22 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:22847 ZCPLUS Full-text
DOCUMENT NUMBER: 86:22847
TITLE: Charged particle spectra from 100 MeV proton on nickel-58
AUTHOR(S): Wu, J. R.; Chang, C. C.; Holmgren, H. D.; Wall, N. S.; Didelez, J. P.; Butterfield, C.
CORPORATE SOURCE: Dep. Phys., Univ. Maryland, College Park, MD, USA
SOURCE: Clustering Phenom. Nucl., Invited Lect. Contrib. Pap. Int. Conf., 2nd (1975), Issue ORO-4856-26, 360-1.
Editor(s): Goldberg, D. A.; Marion, J. B.; Wallace, S. J. NTIS: Springfield, Va.
CODEN: 34GDA8

DOCUMENT TYPE: Conference
LANGUAGE: English

AB Charged particle spectra resulting from 100-MeV p bombardment of 58Ni [13981-79-8] were measured with a triple-counter-telescope. Data are presented on energy spectra at 9 angles, angle-integrated energy spectra, energy-integrated angular distributions, and angular distributions at different energy intervals. The integral emission cross sections for p (excluding elastic peak), d, t, τ , and α were 890 ± 30 , 87 ± 10 , 9 ± 3 , 13 ± 4 , and 120 ± 14 mb, resp. The high-energy angular distributions are anisotropic, indicating preequil. emission, whereas the low-energy distributions are nearly isotropic, suggesting an evaporation process.

CC 70-2 (Nuclear Phenomena)

L23 ANSWER 23 OF 23 ZCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:22837 ZCPLUS Full-text
DOCUMENT NUMBER: 86:22837
TITLE: Quasifree scattering in the $^{24}\text{Mg}(\text{p},\text{p}\alpha)^{20}\text{Ne}$ reaction at 100 MeV
AUTHOR(S): Steinberg, R. I.; Chang, C. C.; Chant, N. S.; Didelez, J. P.; Holmgren, H. D.; Roos, Philip G.; Wu, J. S.
CORPORATE SOURCE: Dep: Phys. Astron., Univ. Maryland, College Park, MD, USA
SOURCE: Clustering Phenom. Nucl., Invited Lect. Contrib. Pap. Int. Conf., 2nd (1975), Issue ORO-4856-26, 315-16.
Editor(s): Goldberg, D. A.; Marion, J. B.; Wallace, S. J. NTIS: Springfield, Va.

CODEN: 34GDA8
DOCUMENT TYPE: Conference
LANGUAGE: English
AB Quasifree scattering data are presented for the $^{24}\text{Mg}(\text{p},\text{p}\alpha)^{20}\text{Ne}$ reaction for 2 pairs of quasifree angles for an incident p energy of 100 MeV.
CC 70-2 (Nuclear Phenomena)

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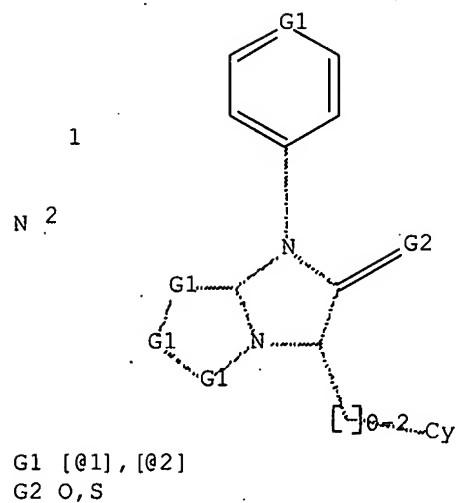
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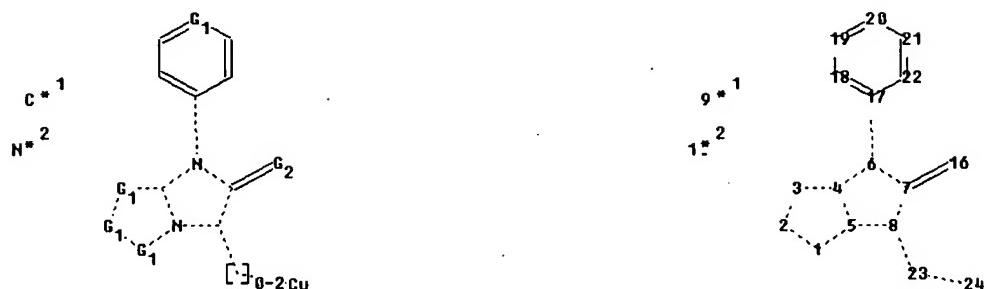
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=> d stat que L20
L1 STR



Structure attributes must be viewed using STN Express query preparation:
 Uploading L1.str



chain nodes :

16 23 24

ring nodes :

1 2 3 4 5 6 7 8 9 10 17 18 19 20 21 22

chain bonds :

6-17 7-16 8-23 23-24

ring bonds :

1-2 1-5 2-3 3-4 4-5 4-6 5-8 6-7 7-8 17-18 17-22 18-19 19-20 20-21 21-22

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5 4-6 5-8 6-7 6-17 7-8 7-16 8-23 17-18 17-22 18-19
19-20 20-21 21-22 23-24

G1:[*1], [*2]

G2:O, S

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS 24:Atom

Generic attributes :

24:

Saturation : Unsaturated

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L34 21 L20 NOT L23

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L34 ANSWER 1 OF 21 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:1070309 ZCPLUS Full-text

DOCUMENT NUMBER: 145:389375

TITLE: Derivatives of [6,7-dihydro-5H-imidazo[1,2-alpha]imidazole-3-sulfonyl]-azetidine-carboxylic acids, esters and amides and use thereof as anti-inflammatory agents

INVENTOR(S): Brunette, Steven Richard

PATENT ASSIGNEE(S): Boehringer Ingelheim International GmbH, Germany;
Boehringer Ingelheim Pharma GmbH & Co. KG

SOURCE: PCT Int. Appl., 52pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006107941	A1	20061012	WO 2006-US12455	20060404
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			

US 2006229287 A1 20061012 US 2006-278579 20060404
 PRIORITY APPLN. INFO.: US 2005-668906P P 20050406
 OTHER SOURCE(S): MARPAT 145:389375

AB Derivs. of [6,7-dihydro-5H-imidazo[1,2-a]imidazole-3-sulfonyl]-azetidine-carboxylic acids, esters and amides which exhibit good inhibitory effect upon the interaction of cell adhesion mols. (CAMs) and leukointegrins and are thus useful in the treatment of inflammatory disease.

IT 911634-16-7P 911634-18-9P 911634-19-0P

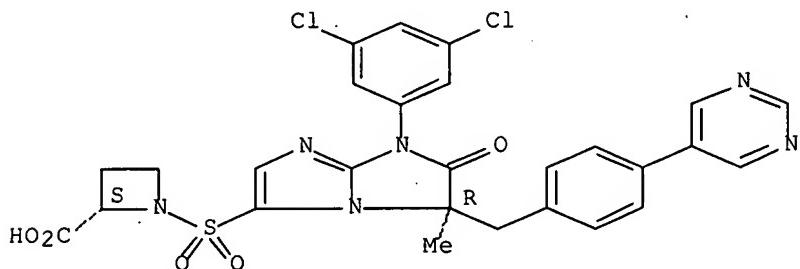
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(derivs. of [dihydro-5H-imidazo[1,2-a]imidazole-3-sulfonyl]-azetidine-carboxylic acids, esters and amides as anti-inflammatory agents and inhibition of cell adhesion mols. interaction with leukointegrins)

RN 911634-16-7 ZCPLUS

CN 2-Azetidinecarboxylic acid, 1-[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-, (2S)- (9CI) (CA INDEX NAME)

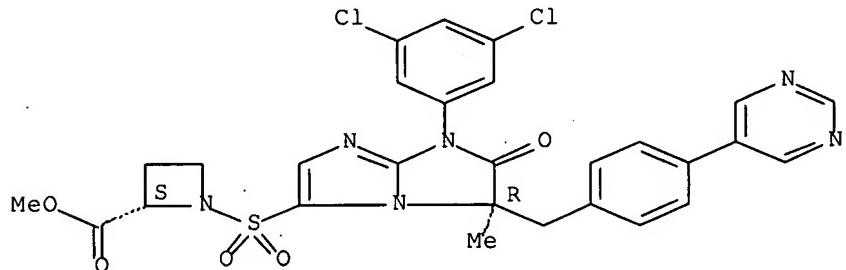
Absolute stereochemistry.



RN 911634-18-9 ZCPLUS

CN 2-Azetidinecarboxylic acid, 1-[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-, methyl ester, (2S)- (9CI) (CA INDEX NAME)

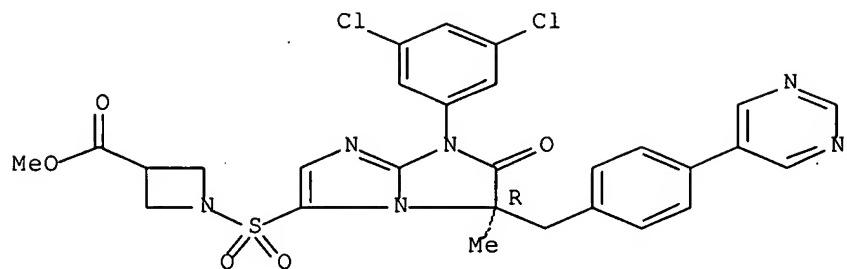
Absolute stereochemistry.



RN 911634-19-0 ZCPLUS

CN 3-Azetidinecarboxylic acid, 1-[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 911634-20-3P 911634-21-4P 911634-22-5P
911634-23-6P 911634-24-7P 911634-25-8P
911634-26-9P 911634-27-0P 911634-28-1P
911634-29-2P 911634-30-5P 911634-31-6P
911634-32-7P 911634-33-8P 911634-34-9P
911634-35-0P 911634-36-1P 911634-37-2P
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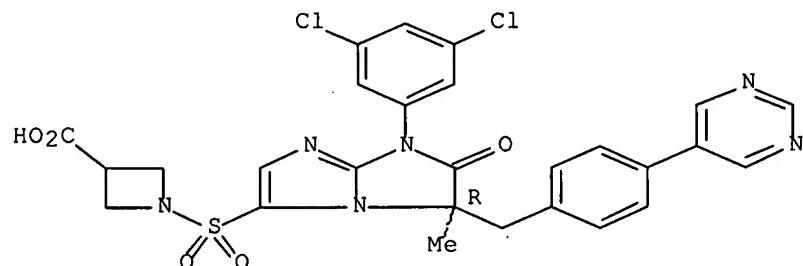
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(derivs. of [dihydro-5H-imidazoimidesulfonyl]-azetidine-carboxylic acids, esters and amides as anti-inflammatory agents and inhibition of cell adhesion mols. interaction with leukointegrins)

RN 911634-20-3 ZCAPLUS

CN 3-Azetidinecarboxylic acid, 1-[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[(4-(5-pyrimidinyl)phenyl)methyl]-1H-imidazo[1,2-a]imidazol-5-ylsulfonyl]- (9CI) (CA INDEX NAME)

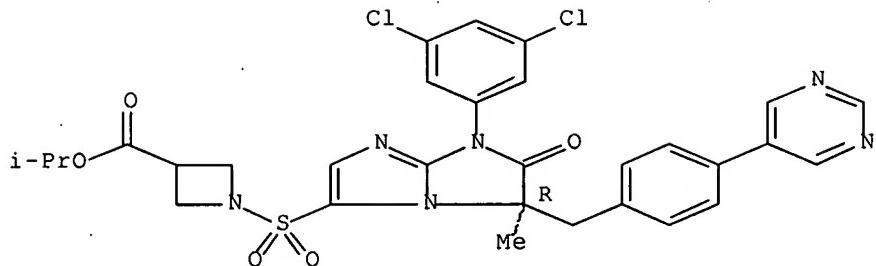
Absolute stereochemistry.



RN 911634-21-4 ZCAPLUS

CN 3-Azetidinecarboxylic acid, 1-[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[(4-(5-pyrimidinyl)phenyl)methyl]-1H-imidazo[1,2-a]imidazol-5-ylsulfonyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

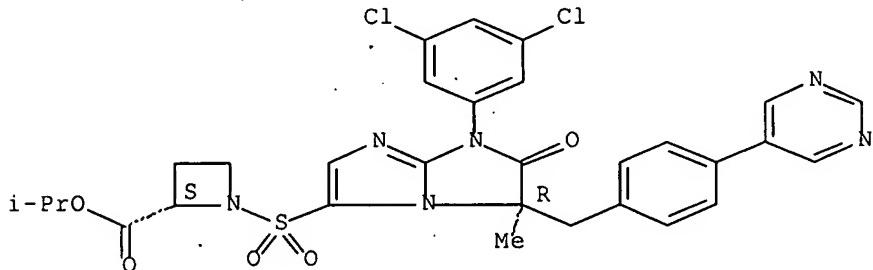
Absolute stereochemistry.



RN 911634-22-5 ZCPLUS

CN 2-Azetidinecarboxylic acid, 1-[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[(4-(5-pyrimidinyl)phenyl)methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-, 1-methylethyl ester, (2S)- (9CI) (CA INDEX NAME)

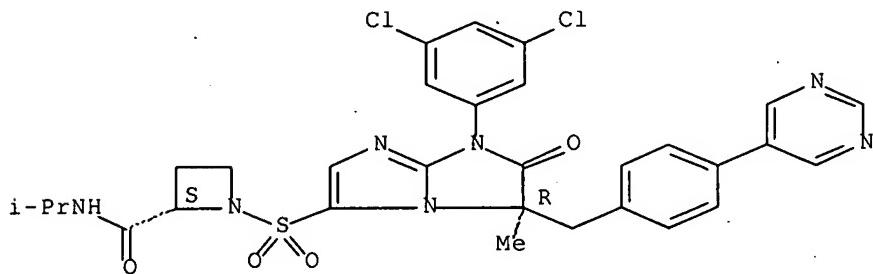
Absolute stereochemistry.



RN 911634-23-6 ZCPLUS

CN 2-Azetidinecarboxamide, 1-[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[(4-(5-pyrimidinyl)phenyl)methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N-(1-methylethyl)-, (2S)- (9CI) (CA INDEX NAME)

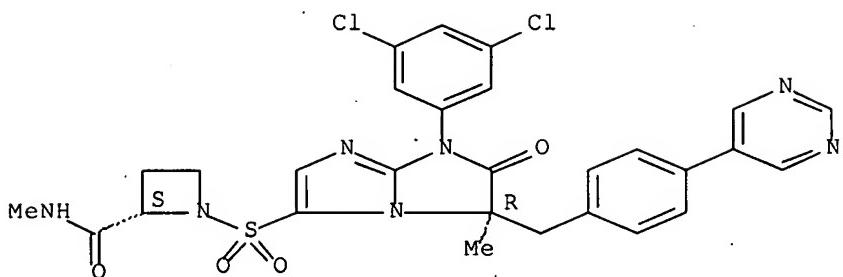
Absolute stereochemistry.



RN 911634-24-7 ZCPLUS

CN 2-Azetidinecarboxamide, 1-[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[(4-(5-pyrimidinyl)phenyl)methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

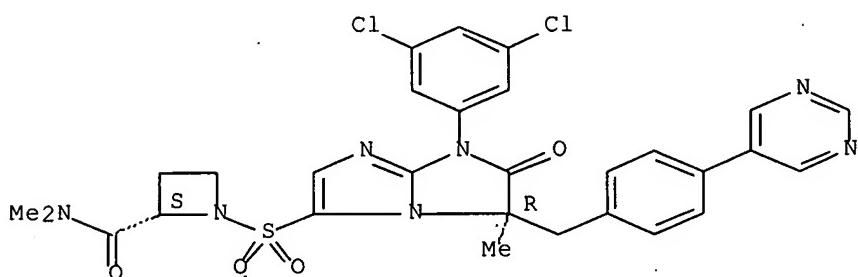
Absolute stereochemistry.



RN 911634-25-8 ZCPLUS

CN 2-Azetidinecarboxamide, 1-[[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[(4-(5-pyrimidinyl)phenyl)methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N,N-dimethyl-, (2S)- (9CI) (CA INDEX NAME)

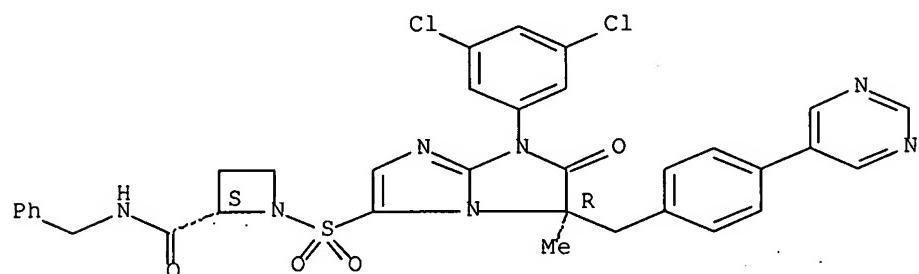
Absolute stereochemistry.



RN 911634-26-9 ZCPLUS

CN 2-Azetidinecarboxamide, 1-[[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[(4-(5-pyrimidinyl)phenyl)methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N-(phenylmethyl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

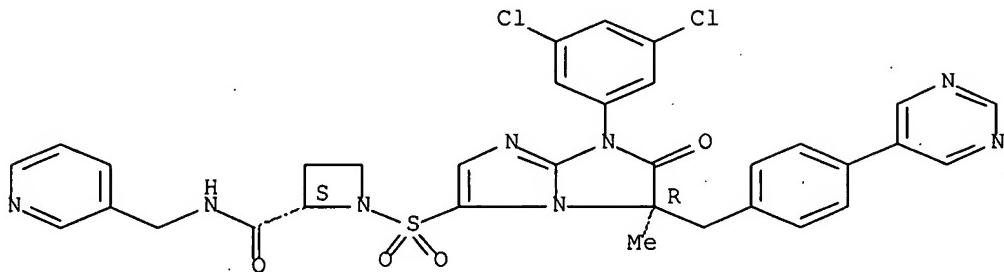


RN 911634-27-0 ZCPLUS

CN 2-Azetidinecarboxamide, 1-[[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[(4-(5-pyrimidinyl)phenyl)methyl]-1H-imidazo[1,2-a]imidazol-

5-yl]sulfonyl]-N-(3-pyridinylmethyl)-, (2S)- (9CI) (CA INDEX NAME)

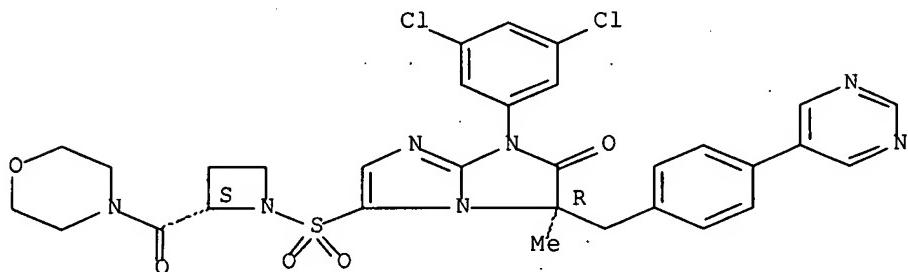
Absolute stereochemistry.



RN 911634-28-1 ZCPLUS

CN Morpholine, 4-[[[(2S)-1-[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[(4-(5-pyrimidinyl)phenyl)methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-2-azetidinyl]carbonyl]- (9CI) (CA INDEX NAME)

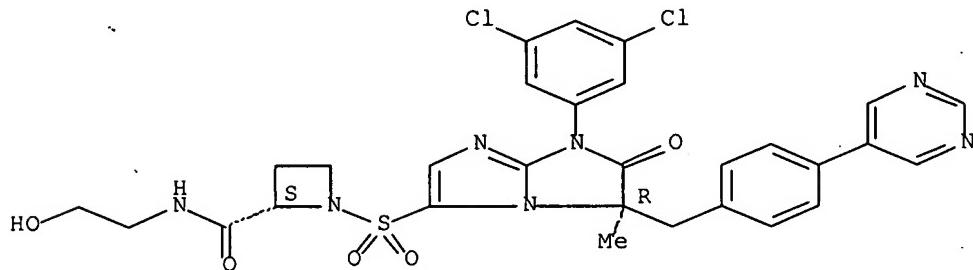
Absolute stereochemistry.



RN 911634-29-2 ZCPLUS

CN 2-Azetidinecarboxamide, 1-[[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[(4-(5-pyrimidinyl)phenyl)methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N-(2-hydroxyethyl)-, (2S)- (9CI) (CA INDEX NAME)

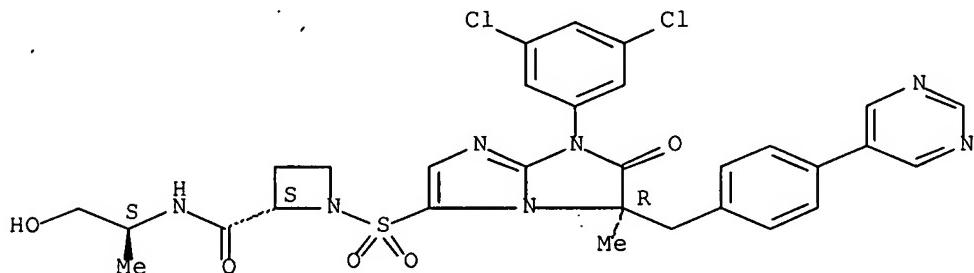
Absolute stereochemistry.



RN 911634-30-5 ZCPLUS

CN 2-Azetidinecarboxamide, 1-[[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N-[(1S)-2-hydroxy-1-methylethyl]-, (2S)- (9CI) (CA INDEX NAME)

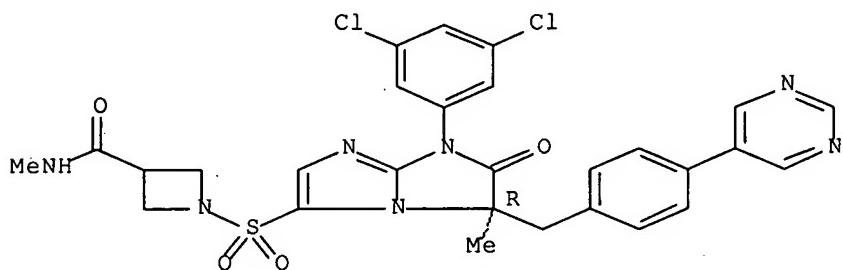
Absolute stereochemistry.



RN 911634-31-6 ZCPLUS

CN 3-Azetidinecarboxamide, 1-[[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N-methyl- (9CI) (CA INDEX NAME)

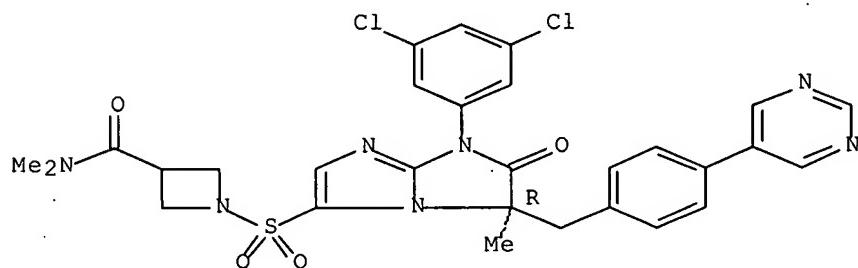
Absolute stereochemistry.



RN 911634-32-7 ZCPLUS

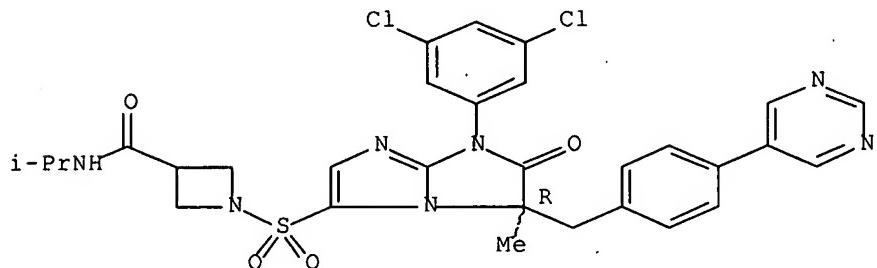
CN 3-Azetidinecarboxamide, 1-[[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



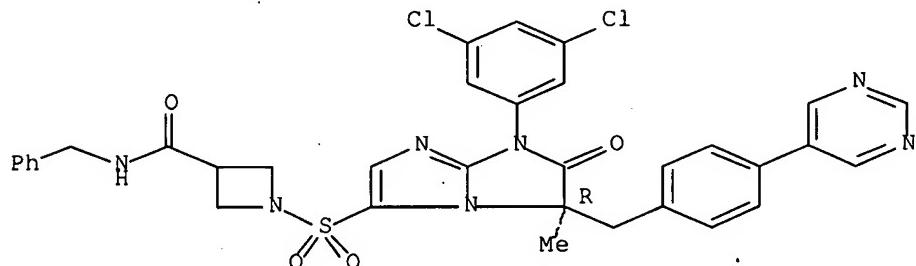
RN 911634-33-8 ZCPLUS
CN 3-Azetidinecarboxamide, 1-[[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



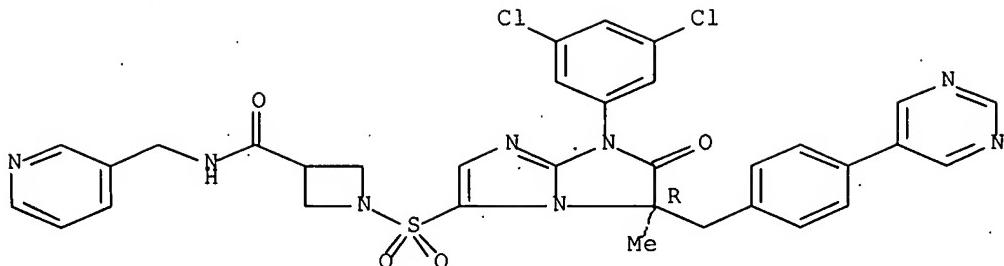
RN 911634-34-9 ZCPLUS
CN 3-Azetidinecarboxamide, 1-[[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 911634-35-0 ZCPLUS
CN 3-Azetidinecarboxamide, 1-[[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

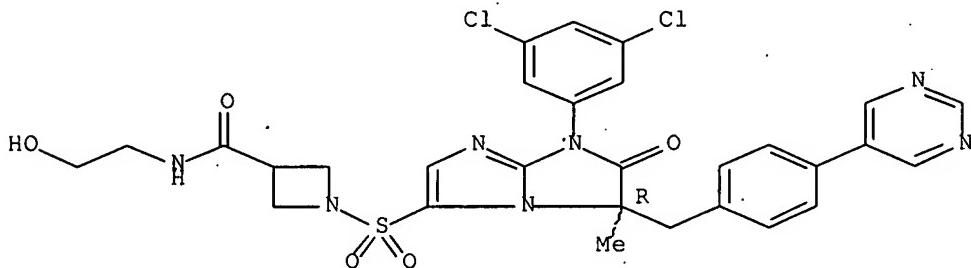
Absolute stereochemistry.



RN 911634-36-1 ZCAPLUS

CN 3-Azetidinecarboxamide, 1-[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-ylsulfonyl]-N-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)

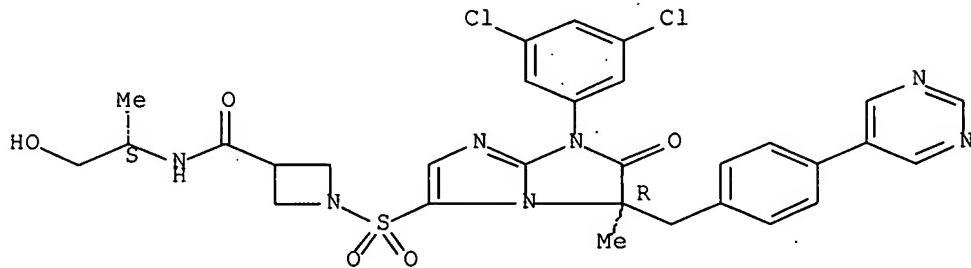
Absolute stereochemistry.



RN 911634-37-2 ZCAPLUS

CN 3-Azetidinecarboxamide, 1-[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[(4-(5-pyrimidinyl)phenyl)methyl]-1H-imidazo[1,2-a]imidazol-5-ylsulfonyl]-N-[(1S)-2-hydroxy-1-methylethyl]- (9CI) (CA INDEX NAME)

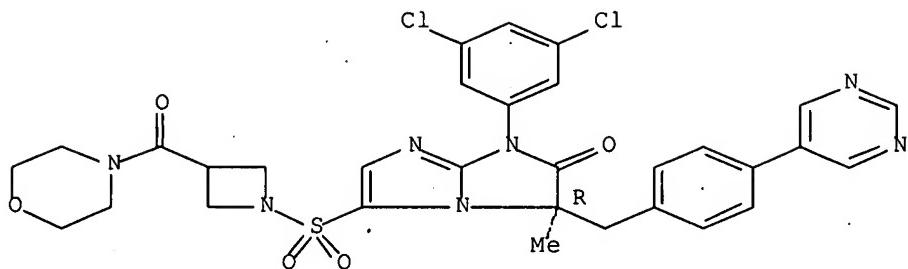
Absolute stereochemistry.



RN 911634-38-3 ZCPLUS

CN Morpholine, 4-[[1-[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-3-azetidinyl]carbonyl]- (9CI) (CA INDEX NAME)

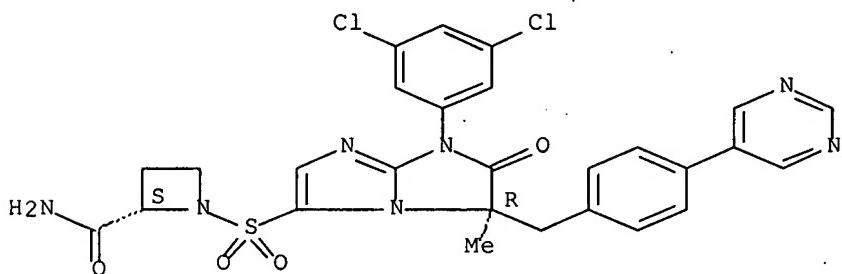
Absolute stereochemistry.



RN 911634-39-4 ZCPLUS

CN 2-Azetidinecarboxamide, 1-[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[(4-(5-pyrimidinyl)phenyl)methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-, (2S)- (9CI) (CA INDEX NAME)

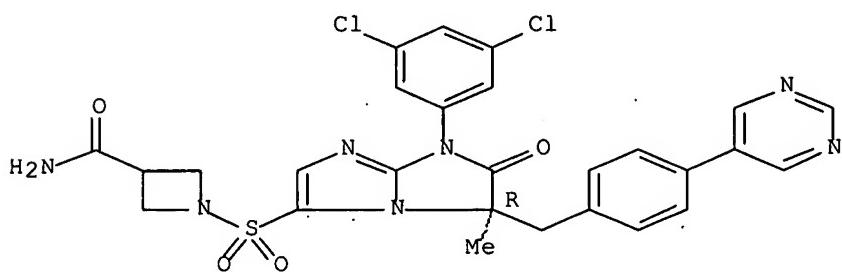
Absolute stereochemistry.



RN 911634-40-7 ZCPLUS

CN 3-Azetidinecarboxamide, 1-[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[(4-(5-pyrimidinyl)phenyl)methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

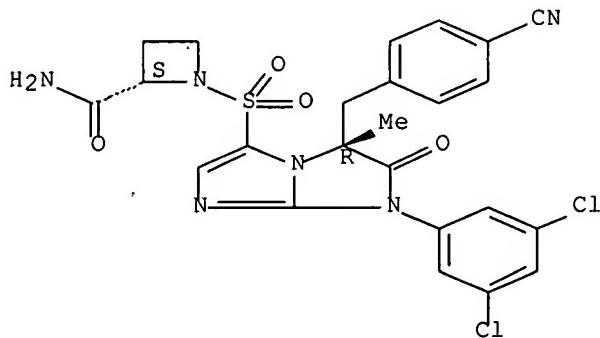


RN 911634-41-8 ZCPLUS

CN 2-Azetidinecarboxamide, 1-[(3R)-3-[(4-cyanophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-

yl]sulfonyl]-, (2S)- (9CI) (CA INDEX NAME)

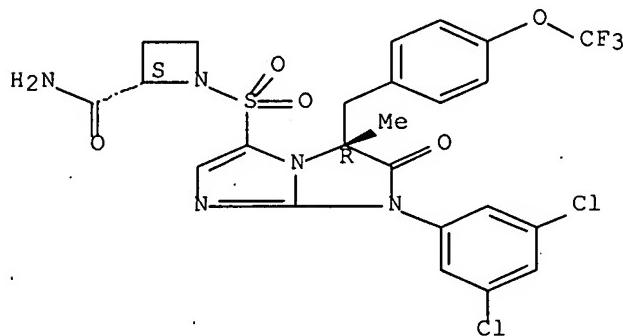
Absolute stereochemistry.



RN 911634-44-1 ZCPLUS

CN 2-Azetidinécarboxamide, 1-[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[(4-(trifluoromethoxy)phenyl)methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-, (2S)- (9CI) (CA INDEX NAME)

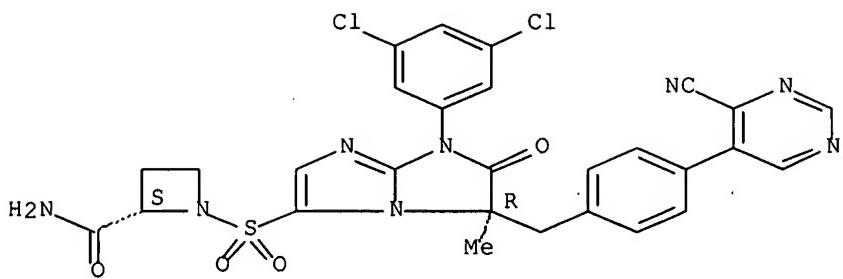
Absolute stereochemistry.



RN 911634-45-2 ZCPLUS

CN 2-Azetidinecarboxamide, 1-[(3R)-3-[(4-(4-cyano-5-pyrimidinyl)phenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



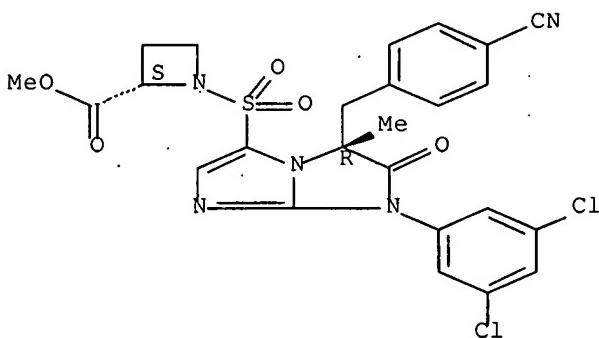
IT 911634-42-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; derivs. of [dihydro-5H-imidazoimidazolesulfonyl]-azetidine-carboxylic acids, esters and amides as anti-inflammatory agents and inhibition of cell adhesion mols. interaction with leukointegrins)

RN 911634-42-9 ZCPLUS

CN 2-Azetidinecarboxylic acid, 1-[(3R)-3-[(4-cyanophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-ylsulfonyl]-, methyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 688756-08-3, (R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazole-3-sulfonyl chloride

688756-19-6, (R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-(4-trifluoromethoxybenzyl)-6,7-dihydro-5H-imidazo[1,2-a]imidazole-3-sulfonyl chloride 911634-17-8 911634-43-0

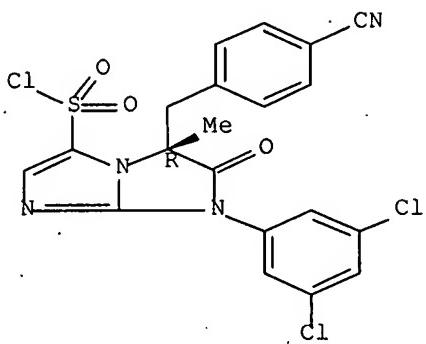
RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant; derivs. of [dihydro-5H-imidazoimidazolesulfonyl]-azetidine-carboxylic acids, esters and amides as anti-inflammatory agents and inhibition of cell adhesion mols. interaction with leukointegrins)

RN 688756-08-3 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazole-5-sulfonyl chloride, 3-[(4-cyanophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-, (3R)- (CA INDEX NAME)

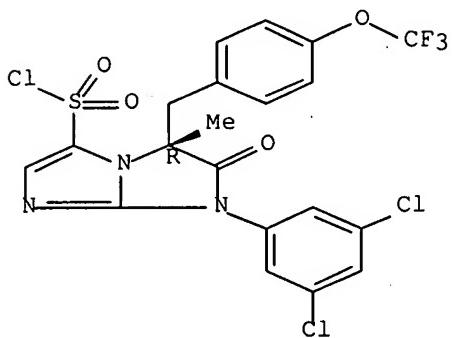
Absolute stereochemistry.



RN 688756-19-6 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazole-5-sulfonyl chloride, 1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[4-(trifluoromethoxy)phenyl]methyl-, (3R)- (CA INDEX NAME)

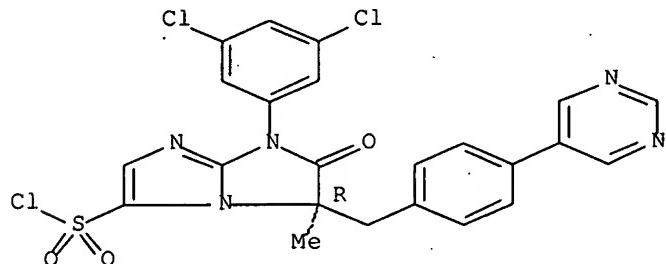
Absolute stereochemistry.



RN 911634-17-8 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazole-5-sulfonyl chloride, 1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[4-(5-pyrimidinyl)phenyl]methyl-, (3R)- (9CI) (CA INDEX NAME)

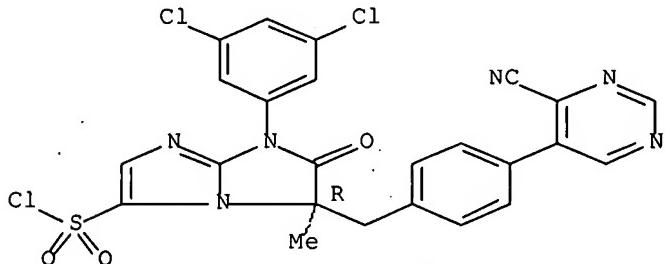
Absolute stereochemistry.



RN 911634-43-0 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazole-5-sulfonyl chloride, 3-[(4-(4-cyano-5-pyrimidinyl)phenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 2 OF 21 ZCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:600124 ZCPLUS Full-text
DOCUMENT NUMBER: 145:230586
TITLE: Mild Iodine-Magnesium Exchange of Iodoaromatics Bearing a Pyrimidine Ring with Isopropylmagnesium Chloride
AUTHOR(S): Wang, Xiao-Jun; Xu, Yibo; Zhang, Li; Krishnamurthy, Dhileepkumar; Senanayake, Chris H.
CORPORATE SOURCE: Department of Chemical Development, Boehringer Ingelheim Pharmaceuticals Inc., Ridgefield, CT, 06877, USA
SOURCE: Organic Letters (2006), 8(14), 3141-3144
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:230586

AB (Iodo)arenes bearing a reactive pyrimidine ring underwent a clean iodine-magnesium exchange with isopropylmagnesium chloride in the presence of bis[2-(dimethylamino)ethyl] ether to provide the corresponding Grignard reagents. The presence of bis[2-(dimethylamino)ethyl] ether prevented reduction of the pyrimidine ring and addition by isopropylmagnesium chloride. As a result, the newly formed reactive Grignard reagents were allowed to react with electrophiles in a highly selective manner to afford adducts in excellent yields.

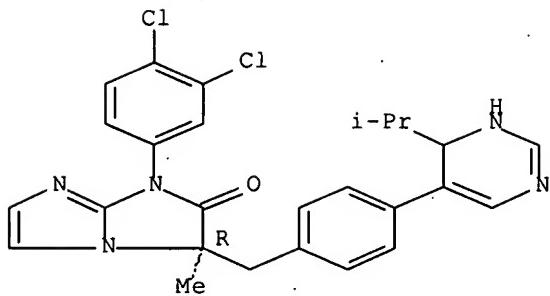
IT 905840-79-1P 905840-80-4P 905840-81-5P

RL: BYP (Byproduct); PREP (Preparation)
(mild iodine-magnesium exchange of chiral iodo(chlorophenyl)methyl[(pyrimidinyl)phenyl]methylimidazo[1,2-a]imidazolone derivs. with isopropylmagnesium chloride)

RN 905840-79-1 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3,5-dichlorophenyl)-3-[(4-[1,4-dihydro-4-(1-methylethyl)-5-pyrimidinyl]phenyl)methyl]-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

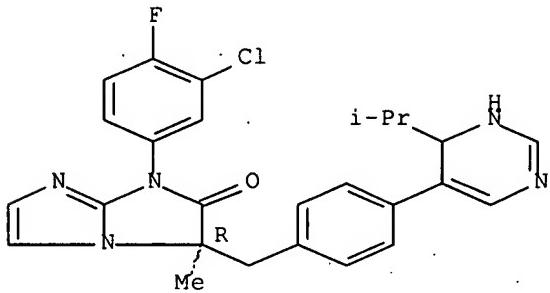
Absolute stereochemistry.



RN 905840-80-4 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3-chloro-4-fluorophenyl)-3-[(4-[1,4-dihydro-4-(1-methylethyl)-5-pyrimidinyl]phenyl)methyl]-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

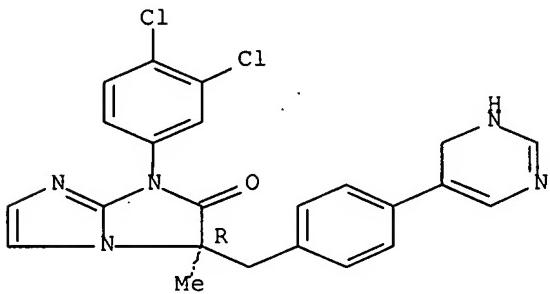
Absolute stereochemistry.



RN 905840-81-5 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3,4-dichlorophenyl)-3-[(4-(1,4-dihydro-5-pyrimidinyl)phenyl)methyl]-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 905840-75-7P, 905840-76-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

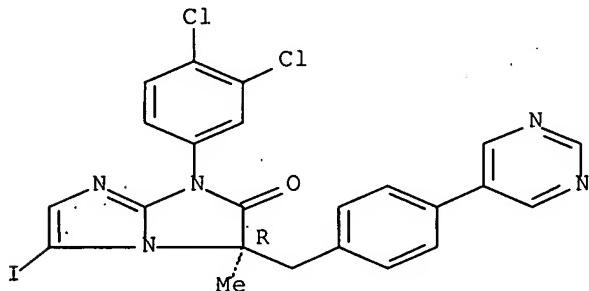
(Reactant or reagent)

(mild iodine-magnesium exchange of chiral iodo(chlorophenyl)methyl[(pyr imidinyl)phenyl]methyl]imidazo[1,2-a]imidazolone derivs. with isopropylmagnesium chloride)

RN 905840-75-7 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3,4-dichlorophenyl)-5-iodo-3- methyl-3-[(4-(5-pyrimidinyl)phenyl)methyl]-, (3R)- (9CI) (CA INDEX NAME)

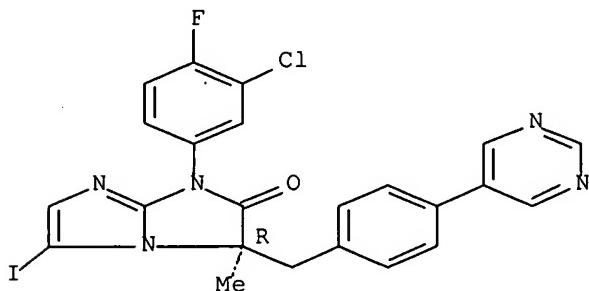
Absolute stereochemistry.



RN 905840-76-8 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3-chloro-4-fluorophenyl)-5-iodo-3- methyl-3-[(4-(5-pyrimidinyl)phenyl)methyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 905840-77-9P 905840-78-0P

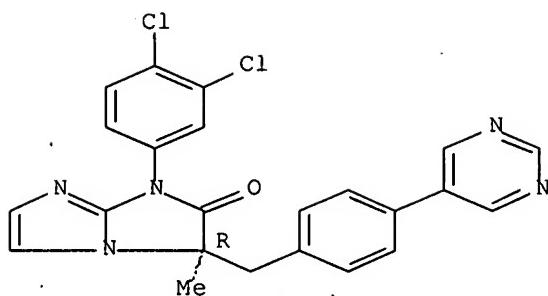
RL: SPN (Synthetic preparation); PREP (Preparation)

(mild iodine-magnesium exchange of chiral iodo(chlorophenyl)methyl[(pyr imidinyl)phenyl]methyl]imidazo[1,2-a]imidazolone derivs. with isopropylmagnesium chloride)

RN 905840-77-9 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3,4-dichlorophenyl)-3-methyl-3-[(4-(5-pyrimidinyl)phenyl)methyl]-, (3R)- (9CI) (CA INDEX NAME)

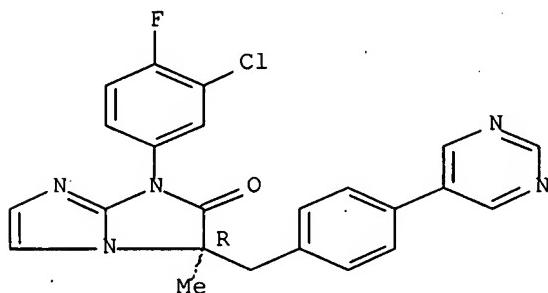
Absolute stereochemistry.



RN 905840-78-0 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3-chloro-4-fluorophenyl)-3-methyl-3-[(4-(5-pyrimidinyl)phenyl)methyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



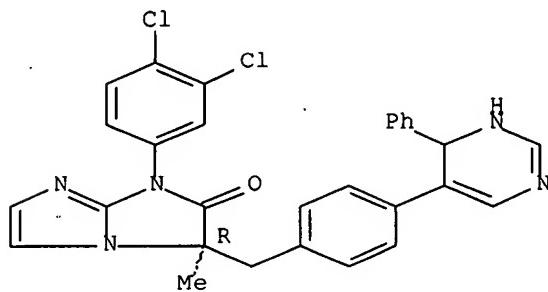
IT 905840-85-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(reaction of chiral iodo(chlorophenyl)methyl[(pyrimidinyl)phenyl]methyl imidazo[1,2-a]imidazolone with phenylmagnesium chloride)

RN 905840-85-9 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3,4-dichlorophenyl)-3-[(4-(1,4-dihydro-4-phenyl-5-pyrimidinyl)phenyl)methyl]-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 3 OF 21 ZCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:104683 ZCPLUS Full-text
DOCUMENT NUMBER: 144:192252
TITLE: Process for preparation of oxoimidazolesulfonamides.
INVENTOR(S): Wang, Xiao-Jun; Wirth, Thomas; Nicola, Thomas; Zhang, Li; Frutos, Rogelio Perez; Xu, Yibo; Krishnamurihy, Dhileopkumar; Nummy, Laurence John; Varsolona, Richard J.; Senanayake, Chris Hugh; Kroeber, Jutta
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA; Boehringer Ingelheim International G.m.b.H.
SOURCE: U.S. Pat. Appl. Publ., 24 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

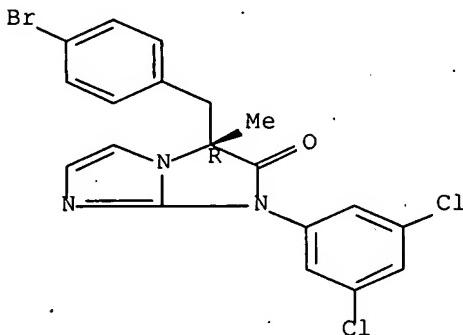
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006025447	A1	20060202	US 2005-188377	20050725
AU 2005269634	A1	20060209	AU 2005-269634	20050725
CA 2573398	A1	20060209	CA 2005-2573398	20050725
WO 2006014828	A1	20060209	WO 2005-US26148	20050725
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP 1776367	A1	20070425	EP 2005-775277	20050725
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BA, HR, YU				
IN 2007DN00045	A	20070427	IN 2007-DN45	20070102
PRIORITY APPLN. INFO.:			US 2004-591398P	P 20040727
			WO 2005-US26148	W 20050725
OTHER SOURCE(S): GI	CASREACT 144:192252; MARPAT 144:192252			

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. [I; R1 = Br, F3CO, cyano, (amino-substituted) pyrimidin-5-yl; Q = R2R3NSO2; .R2, R3 = H, (substituted) alkyl; R2R3N = (substituted) pyrrolidinyl, piperidinyl], were prepared by treatment of I (R1 as above; Q = halo) with an alkylmagnesium halide, SO2, N-chlorosuccinimide, and R2R3NH. Thus, title compound (II) was prepared in 75% yield by treatment of the

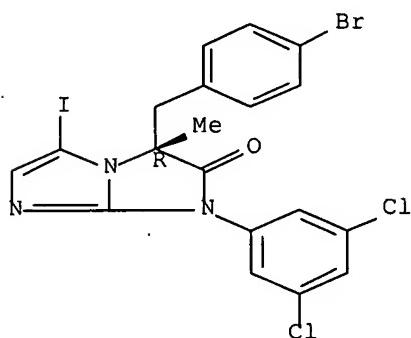
corresponding iodide with isopropylmagnesium
 chloride/tetramethylethylenediamine/SO₂/N-chlorosuccinimide/isonipecotamide
 e/diisopropylethylamine in THF at -20° to 22°.
 IT 321656-72-8P 321656-73-9P 321720-72-3P
 321722-94-5P 875210-71-2P 875210-72-3P
 875210-76-7P 875210-77-8P
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
 preparation); PREP (Preparation); RACT (Reactant or reagent)
 (process for preparation of dihydroooimidazolesulfonamides)
 RN 321656-72-8 ZCPLUS
 CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 3-[(4-bromophenyl)methyl]-1-(3,5-
 dichlorophenyl)-3-methyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



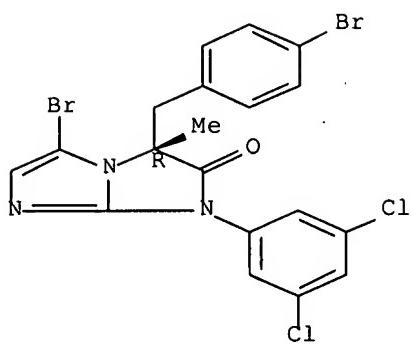
RN 321656-73-9 ZCPLUS
 CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 3-[(4-bromophenyl)methyl]-1-(3,5-
 dichlorophenyl)-5-iodo-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 321720-72-3 ZCPLUS
 CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 5-bromo-3-[(4-bromophenyl)methyl]-1-
 (3,5-dichlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

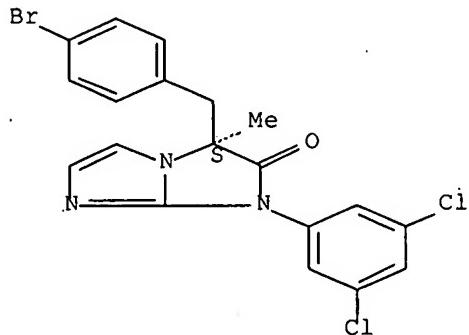
Absolute stereochemistry.



RN 321722-94-5 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-3-methyl-, (3S)- (9CI) (CA INDEX NAME)

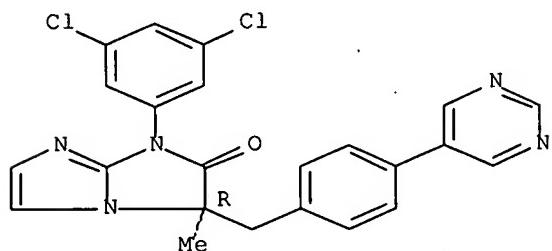
Absolute stereochemistry.



RN 875210-71-2 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3,5-dichlorophenyl)-3-methyl-3-[(4-(5-pyrimidinyl)phenyl)methyl]-, (3R)- (9CI) (CA INDEX NAME)

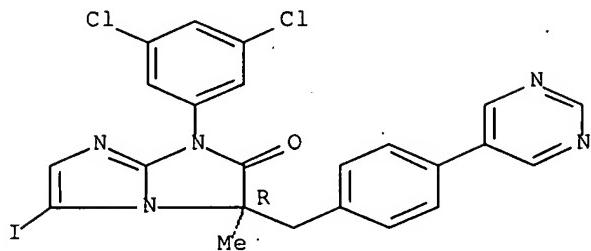
Absolute stereochemistry.



RN 875210-72-3 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3,5-dichlorophenyl)-5-iodo-3-methyl-3-[(4-(5-pyrimidinyl)phenyl)methyl]-, (3R)- (9CI) (CA INDEX NAME)

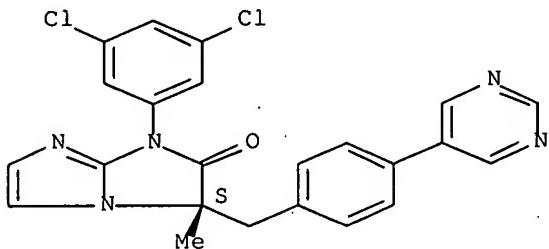
Absolute stereochemistry.



RN 875210-76-7 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3,5-dichlorophenyl)-3-methyl-3-[(4-(5-pyrimidinyl)phenyl)methyl]-, (3S)- (9CI) (CA INDEX NAME)

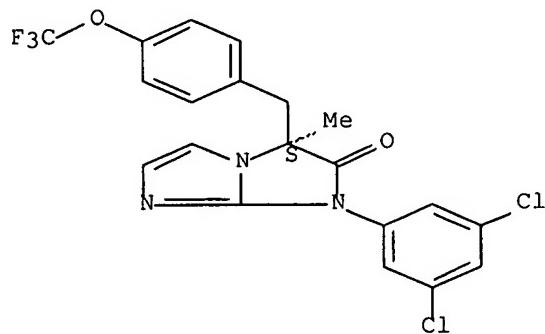
Absolute stereochemistry.



RN 875210-77-8 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3,5-dichlorophenyl)-3-methyl-3-[(4-(trifluoromethoxy)phenyl)methyl]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 321656-57-9P 321656-61-5P 321718-99-4P

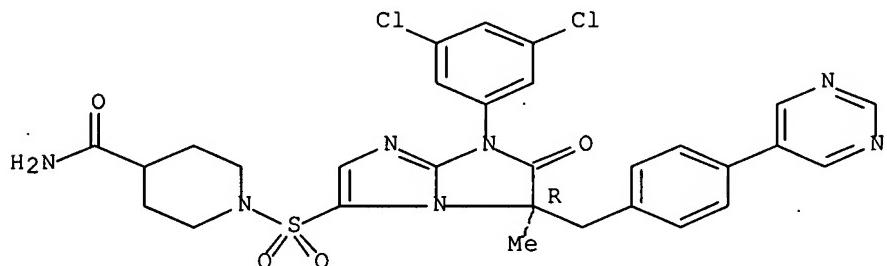
688756-00-5P 875210-67-6P 875210-75-6P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(process for preparation of dihydrooxoimidazoimidazole sulfonamides)

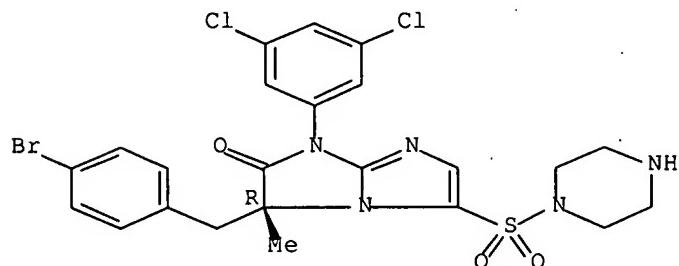
RN 321656-57-9 ZCPLUS
CN 4-Piperidinecarboxamide, 1-[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



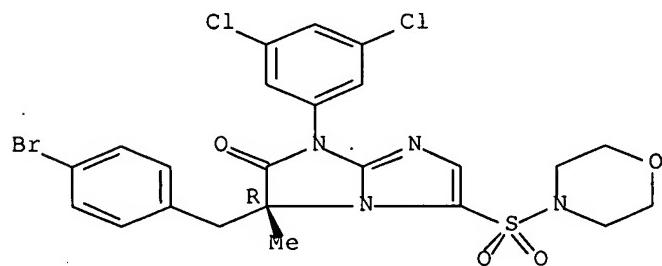
RN 321656-61-5 ZCPLUS
CN Piperazine, 1-[(3R)-3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



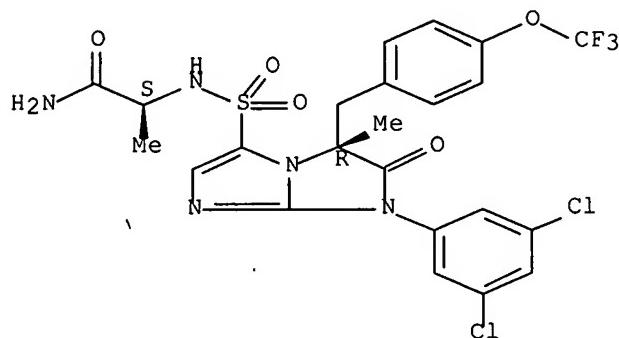
RN 321718-99-4 ZCPLUS
CN Morpholine, 4-[(3R)-3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



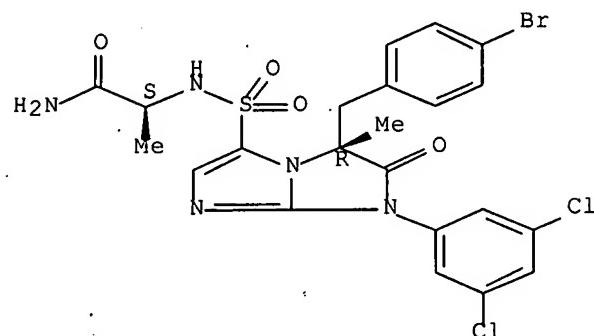
RN 688756-00-5 ZCPLUS
CN Propanamide, 2-[[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(trifluoromethoxy)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



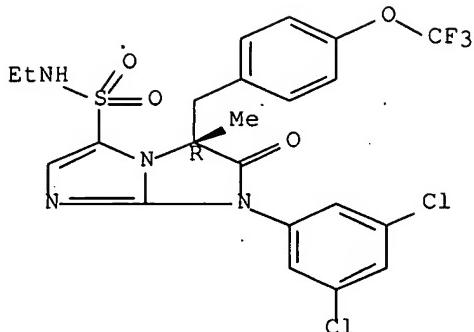
RN 875210-67-6 ZCPLUS
CN Propanamide, 2-[[[(3R)-3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 875210-75-6 ZCPLUS
CN 1H-Imidazo[1,2-a]imidazole-5-sulfonamide, 1-(3,5-dichlorophenyl)-N-ethyl-2,3-dihydro-3-methyl-2-oxo-3-[[4-(trifluoromethoxy)phenyl]methyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L34 ANSWER 4 OF 21 ZCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2005:177881 ZCPLUS Full-text
 DOCUMENT NUMBER: 142:274025
 TITLE: Methods using a combination of a p38 MAP kinase inhibitor with another active agent for the treatment of chronic obstructive pulmonary disease (COPD) and pulmonary hypertension
 INVENTOR(S): Gupta, Abhya; Iacono, Philippe Didier; Kelash-Cannavo, Linda Jean; Madwed, Jeffrey B.; Park, Jung-Yong; Way, Susan Lynn; Yazdanian, Mehran
 PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA; Boehringer Ingelheim Pharma GmbH & Co. KG; Boehringer Ingelheim France S.A.S.
 SOURCE: PCT Int. Appl., 60 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005018624	A2	20050303	WO 2004-US27013	20040819
WO 2005018624	A3	20050506		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004266719	A1	20050303	AU 2004-266719	20040819
CA 2536293	A1	20050303	CA 2004-2536293	20040819
US 2005148555	A1	20050707	US 2004-921448	20040819
EP 1658060	A2	20060524	EP 2004-781654	20040819
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1838958	A	20060927	CN 2004-80024151	20040819
BR 2004013757	A	20061031	BR 2004-13757	20040819

JP 2007503393	T 20070222	JP 2006-524065	20040819
PRIORITY APPLN. INFO.:		US 2003-497376P	P 20030822
		WO 2004-US27013	W 20040819

AB Methods are disclosed for treating COPD and pulmonary hypertension using p38 MAP Kinase inhibitors in combination with one or more other active ingredients.

IT 321656-57-9

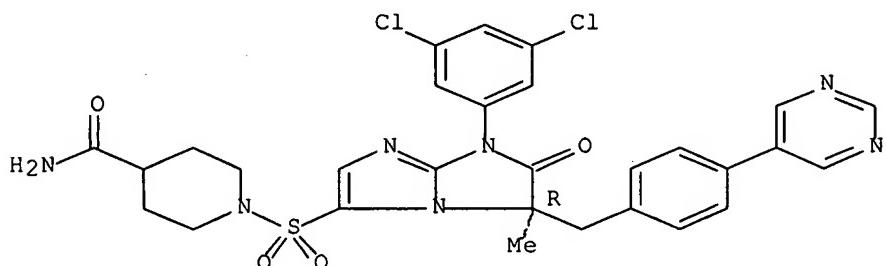
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(p38 MAP kinase inhibitor combination with another active agent for treatment of chronic obstructive pulmonary disease and pulmonary hypertension)

RN 321656-57-9 ZCPLUS

CN 4-Piperidinocarboxamide, 1-[[[3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L34 ANSWER 5 OF 21 ZCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2005:41390 ZCPLUS Full-text
 DOCUMENT NUMBER: 142:299796
 TITLE: Development of a Scalable Process for
 1-(3,5-Dichlorophenyl)-5-iodo-3-methyl-
 (4-methylbenzyl)-1H-imidazo[1,2-a]imidazol-2-one: A
 Key Intermediate for the Synthesis of LFA-1 Inhibitors
 Frutos, Rogelio P.; Eriksson, Magnus; Wang, Xiao-Jun;
 Byrne, Denis; Varsolona, Richard; Johnson, Michael D.;
 Nummy, Lawrence; Krishnamurthy, Dhileepkumar;
 Senanayake, Chris H.
 AUTHOR(S):
 CORPORATE SOURCE: Department of Chemical Development, Boehringer
 Ingelheim Pharmaceuticals, Inc., Ridgefield, CT,
 06877-0368, USA
 SOURCE: Organic Process Research & Development (2005), 9(2),
 137-140
 CODEN: OPRDFK; ISSN: 1083-6160
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 142:299796
 AB A safe, robust, chromatog.-free and reproducible process for the multi-kilogram synthesis of 3-(4-bromobenzyl)-1-(3,5-dichlorophenyl)-5- iodo-3-methyl-1H-imidazo[1,2-a]imidazol-2-one, a key intermediate for the synthesis of LFA-1 inhibitors, was developed and implemented at pilot plant scale. The process allowed support of preclin. activities in the LFA-1 program. Major

improvements were realized by lowering the reaction temperature to -15° and changing the solvent from dichloromethane to acetonitrile, and using TMSI/NaI as reagent system for regioselective hydroiodination. Under the improved conditions, the HI catalyzed proto-deiodination pathway of the intermediate was minimized and the intermediate was obtained in high yield and with low impurity profile.

IT 397329-88-3P 397329-89-4P

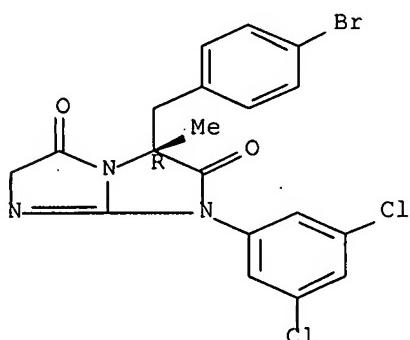
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; pilot-scale process for preparation of dichlorophenyliodo-methylbenzylimidazolimidazolone key intermediate for synthesis of LFA-1 inhibitors)

RN 397329-88-3 ZCAPLUS

CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

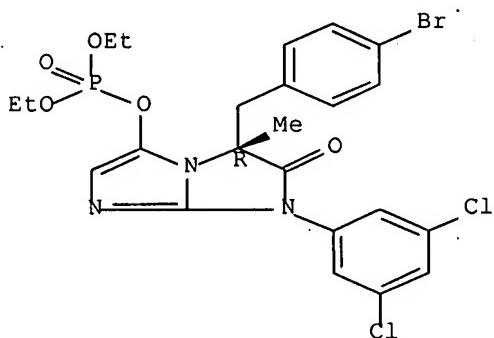
Absolute stereochemistry.



RN 397329-89-4 ZCAPLUS

CN Phosphoric acid, (3R)-3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 321656-73-9P

RL: IMF (Industrial manufacture); PREP (Preparation)

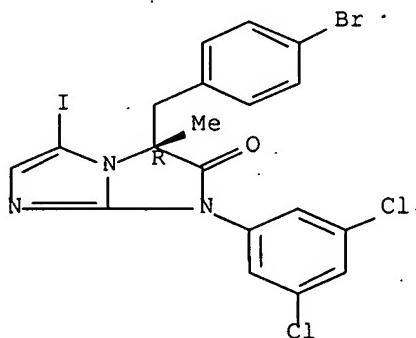
(pilot-scale process for preparation of dichlorophenyliodo-

methylbenzylimidazoimidazolone key intermediate for synthesis of LFA-1
inhibitors)

RN 321656-73-9 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-5-iodo-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 6 OF 21 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:39714 ZCPLUS Full-text

DOCUMENT NUMBER: 143:386961

TITLE: A practical synthesis of highly functionalized fused 1,6-dihydroimidazo[1,2-a]imidazole-2,5-diones, key intermediates for LFA-1 inhibitors. [Erratum to document cited in CA142:197976]

AUTHOR(S): Wang, Xiao-jun; Xu, Yibo; Zhang, Li; Krishnamurthy, Dhileepkumar; Nummy, Laurence; Farina, Vittorio; Senanayake, Chris H.

CORPORATE SOURCE: Department of Chemical Development, Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT, 06877, USA

SOURCE: Synlett (2005), (1), 186
CODEN: SYNLES; ISSN: 0936-5214

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The structures of compound 7 in Scheme 1 and compound 9 in Scheme 4 were incorrectly shown; the corrected Schemes 1 and 4 are given.

IT 397329-88-3P 839678-17-0P 839678-18-1P

839678-19-2P 839678-20-5P 839678-21-6P

839678-22-7P

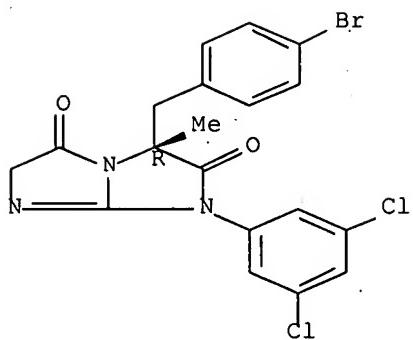
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of functionalized fused 1,6-dihydroimidazo[1,2-a]imidazole-2,5-

diones as key intermediates for LFA-1 inhibitors (Erratum))

RN 397329-88-3 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

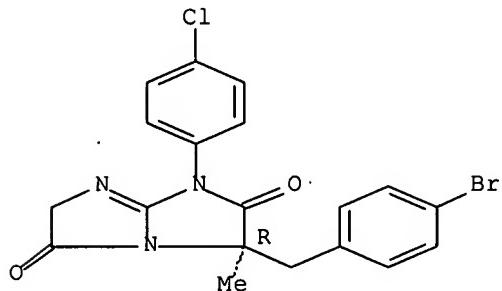
Absolute stereochemistry.



RN 839678-17-0 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-(4-chlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

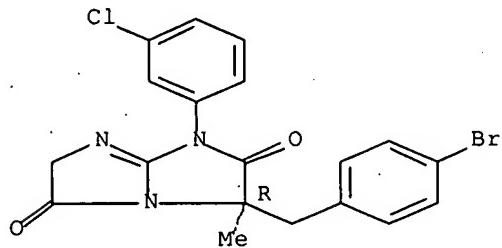
Absolute stereochemistry.



RN 839678-18-1 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-(3-chlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

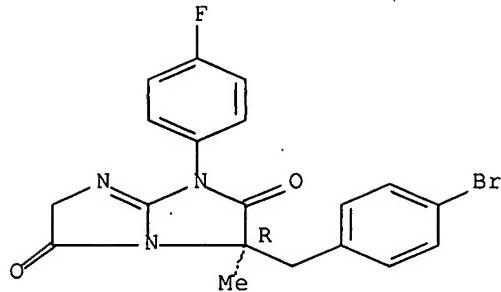
Absolute stereochemistry.



RN 839678-19-2 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-(4-fluorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

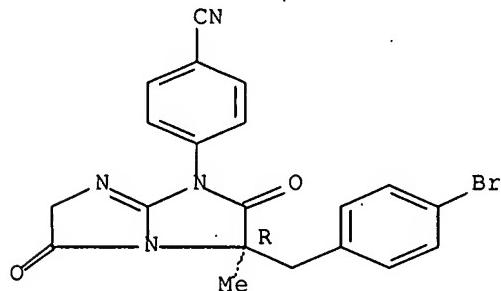
Absolute stereochemistry.



RN 839678-20-5 ZCPLUS

CN Benzonitrile, 4-[(3R)-3-[(4-bromophenyl)methyl]-2,3,5,6-tetrahydro-3-methyl-2,5-dioxo-1H-imidazo[1,2-a]imidazol-1-yl]- (9CI) (CA INDEX NAME)

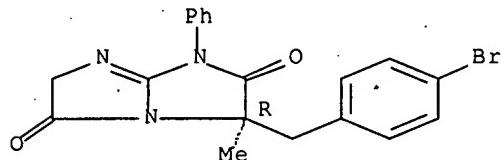
Absolute stereochemistry.



RN 839678-21-6 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-3-methyl-1-phenyl-, (3R)- (9CI) (CA INDEX NAME)

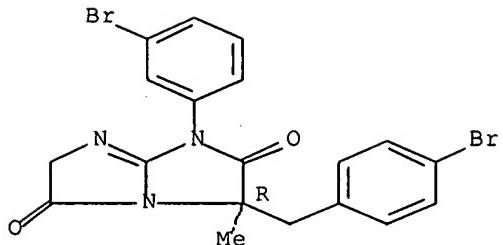
Absolute stereochemistry.



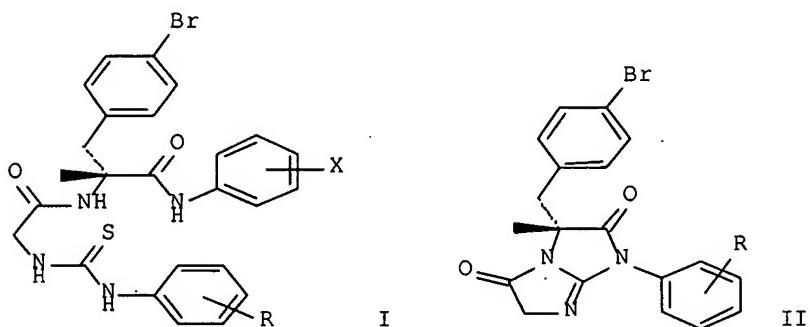
RN 839678-22-7 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 1-(3-bromophenyl)-3-[(4-bromophenyl)methyl]-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L34 ANSWER 7 OF 21 ZCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:1128066 ZCPLUS Full-text
 DOCUMENT NUMBER: 142:197976
 TITLE: A practical synthesis of highly functionalized fused 1,6-dihydroimidazo[1,2-a]imidazole-2,5-diones, key intermediates for LFA-1 inhibitors
 AUTHOR(S): Wang, Xiao-jun; Xu, Yibo; Zhang, Li; Krishnamurthy, Dhileepkumar; Nummy, Laurence; Farina, Vittorio; Senanayake, Chris H.
 CORPORATE SOURCE: Department of Chemical Development, Boehringer Ingelheim Pharmaceuticals Inc., Ridgefield, CT, 06877, USA
 SOURCE: Synlett (2004), (15), 2800-2802
 CODEN: SYNLES; ISSN: 0936-5214
 PUBLISHER: Georg Thieme Verlag
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 142:197976
 GI



- AB An alternative and chromatog.-free approach for synthesis of a new class of LFA-1 inhibitors was developed. A key feature of this process involved a transformation of thioureas I ($X = 3,5\text{-Cl}_2, 4\text{-Cl}$; $R = 4\text{-Cl}, \text{H}, 3\text{-Cl}$, etc.) to acyclic guanidine derivs., followed by intramol. cyclization to highly functionalized bicyclic guanidines II, that were subsequently converted to 1*H*-imidazo[1,2-a]imidazol-2-one LFA-1 inhibitors.
- IT 397329-88-3P 839678-17-0P 839678-18-1P
 839678-19-2P 839678-20-5P 839678-21-6P
 839678-22-7P

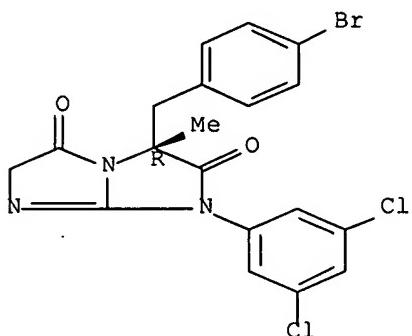
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of functionalized fused 1,6-dihydroimidazo[1,2-a]imidazole-
2,5-

diones as key intermediates for LFA-1 inhibitors)

RN 397329-88-3 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-
(3,5-dichlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

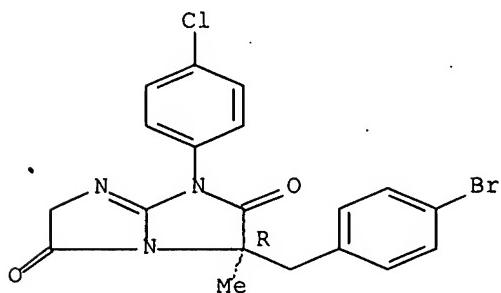
Absolute stereochemistry.



RN 839678-17-0 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-
(4-chlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

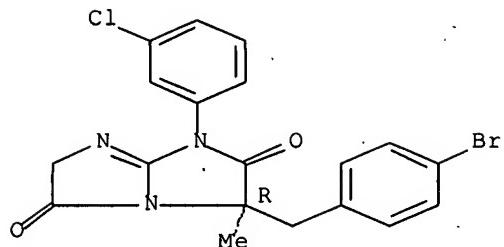
Absolute stereochemistry.



RN 839678-18-1 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-
(3-chlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

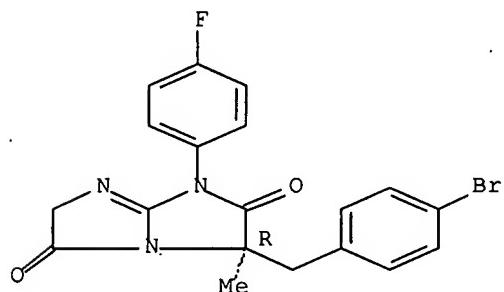
Absolute stereochemistry.



RN 839678-19-2 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-(4-fluorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

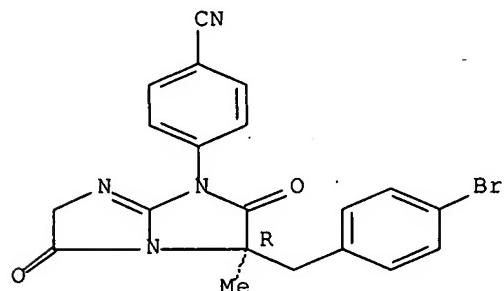
Absolute stereochemistry.



RN 839678-20-5 ZCPLUS

CN Benzonitrile, 4-[(3R)-3-[(4-bromophenyl)methyl]-2,3,5,6-tetrahydro-3-methyl-2,5-dioxo-1H-imidazo[1,2-a]imidazol-1-yl]- (9CI) (CA INDEX NAME)

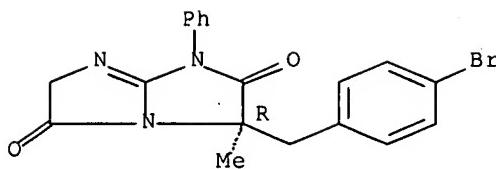
Absolute stereochemistry.



RN 839678-21-6 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-3-methyl-1-phenyl-, (3R)- (9CI) (CA INDEX NAME)

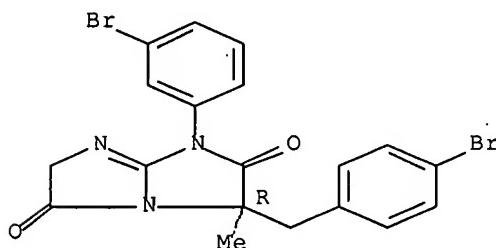
Absolute stereochemistry.



RN 839678-22-7 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 1-(3-bromophenyl)-3-[(4-bromophenyl)methyl]-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 8 OF 21 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:1068436 ZCPLUS Full-text

DOCUMENT NUMBER: 142:197972

TITLE: A practical synthesis of LFA-1 inhibitors utilizing CuCl-promoted intramolecular cyclization of thiohydantoins

AUTHOR(S): Wang, Xiao-jun; Zhang, Li; Xu, Yibo; Krishnamurthy, Dhileepkumar; Varsolona, Richard; Nummy, Laurence; Shen, Sherry; Frutos, Rogelio P.; Byrne, Denis; Chung, J. C.; Farina, Vittorio; Senanayake, Chris H.

CORPORATE SOURCE: Chemical Development Department, Boehringer Ingelheim Pharmaceuticals Inc., Ridgefield, CT, 06877-0368, USA

SOURCE: Tetrahedron Letters (2005), 46(2), 273-276

CODEN: TELEAY; ISSN: 0040-4039

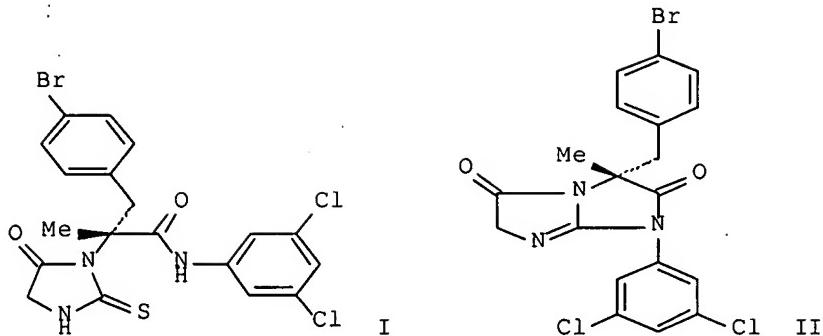
PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:197972

GI



AB An efficient and chromatog.-free approach for synthesis of a new class of LFA-1 (antigen) inhibitors was developed. These compds. are potential inflammation inhibitors (no data). A copper(I) chloride-promoted intramol. cyclization of thiohydantoins serves as a key step to highly functionalized bicyclic guanidines, that were subsequently converted to 1H-imidazo[1,2-a]imidazol-2-one LFA-1 inhibitors. This process has been successfully implemented in the pilot plant to produce multi-kilogram quantities of 1H-imidazo[1,2-a]imidazol-2-one LFA-1 inhibitors. The copper chloride (CuCl)-mediated cyclization of a thiourea derivative (I) gave (3R)-3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-3-methyl-1H-imidazo[1,2-a]imidazole-2,5(3H,6H)-dione (II) in 85-92% yield.

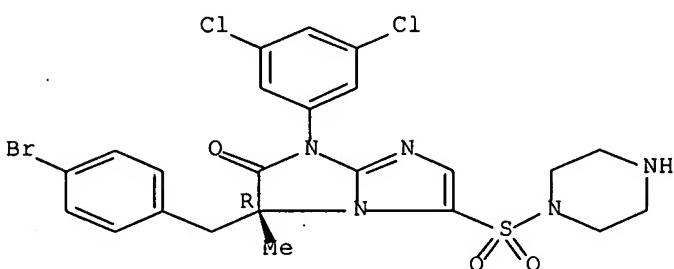
IT 321656-61-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of [(R)-
[(bromophenyl)methyl][di(chloro)phenyl]dihydro(methyl)
(oxo)imidazo[1,2-a]imidazolylsulfonyl]piperazine (bicyclic guanidine)
using copper chloride-promoted cyclization of thiourea derivative as key
synthetic step)

RN 321656-61-5 ZCAPLUS

CN Piperazine, 1-[(3R)-3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-ylsulfonyl]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



IT 321656-62-6P

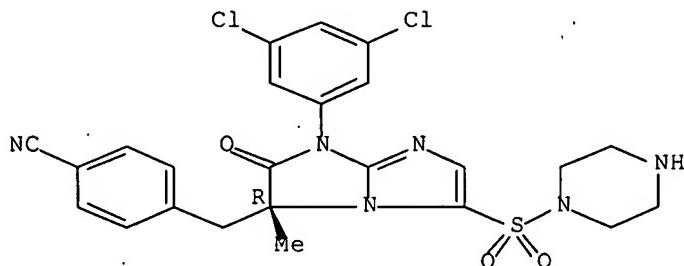
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of [(R)-
[(di(chloro)phenyl)dihydro(methyl)(oxo)[(piperazinyl)sulfonyl]imidazo[1,2-a]imidazolyl]methyl]benzonitrile (bicyclic

guanidine) using copper chloride-promoted cyclization of thiourea derivative as key synthetic step)

RN 321656-62-6 ZCPLUS

CN Piperazine, 1-[(3R)-3-[(4-cyanophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 321656-73-9P 321724-08-7P 397329-88-3P
397329-89-4P 835917-16-3P 835917-17-4P

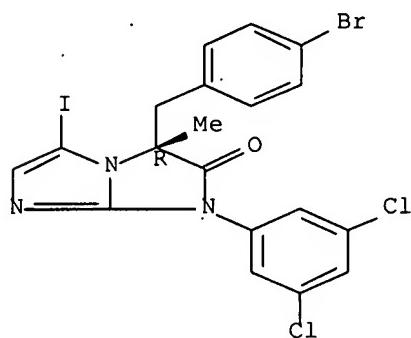
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of [di(chlorophenyl)(methyl)imidazo[1,2-a]imidazoledione (bicyclic guanidine) using copper chloride-promoted cyclization of N-[di(chlorophenyl)(oxo)(thioxo)imidazolidineethanamide (thiourea derivative) as key synthetic step)

RN 321656-73-9 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-5-iodo-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

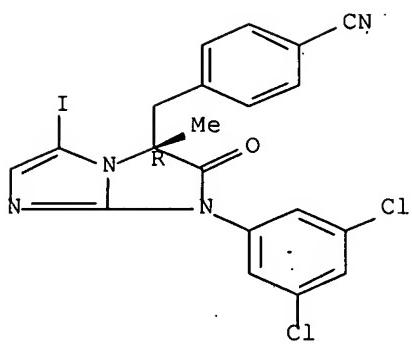
Absolute stereochemistry.



RN 321724-08-7 ZCPLUS

CN Benzonitrile, 4-[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-5-iodo-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-3-ylmethyl]- (CA INDEX NAME)

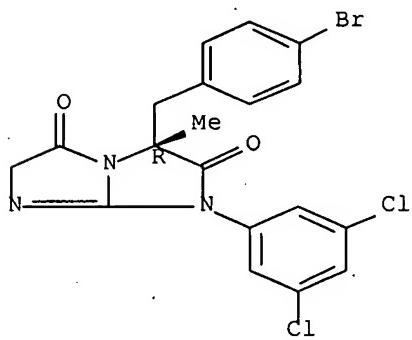
Absolute stereochemistry.



RN 397329-88-3 ZCAPLUS

CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

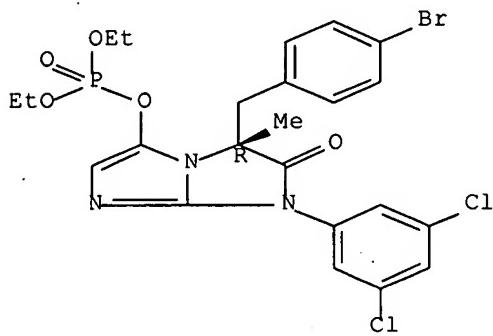
Absolute stereochemistry.



RN 397329-89-4 ZCAPLUS

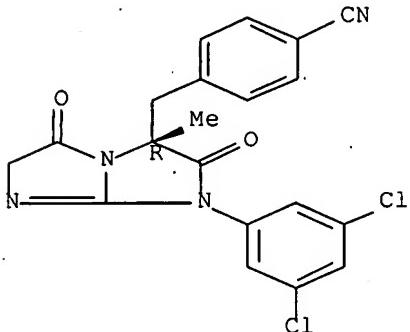
CN Phosphoric acid, (3R)-3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



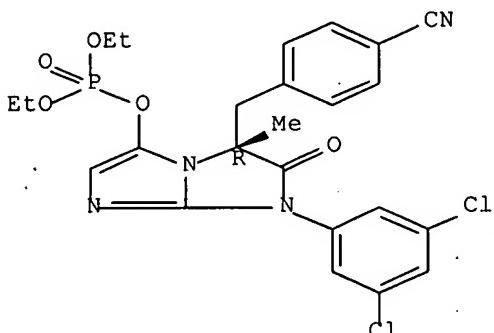
RN 835917-16-3 ZCPLUS
CN Benzonitrile, 4-[(3R)-1-(3,5-dichlorophenyl)-2,3,5,6-tetrahydro-3-methyl-2,5-dioxo-1H-imidazo[1,2-a]imidazol-3-yl]methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 835917-17-4 ZCPLUS
CN Phosphoric acid, (3R)-3-[(4-cyanophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 9 OF 21 ZCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:817893 ZCPLUS Full-text
DOCUMENT NUMBER: 141:332191
TITLE: Preparation of new bicyclic arylimidazolones with nootropic action
INVENTOR(S): Farina, Carlo; Gagliardi, Stefania; Parini, Carlo;
Martinelli, Marisa; Ghelardini, Carla
PATENT ASSIGNEE(S): Nikem Research S.r.l., Italy
SOURCE: PCT Int. Appl., 36 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

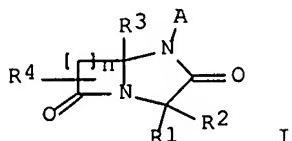
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004085438	A2	20041007	WO 2004-EP50339	20040322
WO 2004085438	A3	20041125		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004224087	A1	20041007	AU 2004-224087	20040322
CA 2520008	A1	20041007	CA 2004-2520008	20040322
EP 1608655	A2	20051228	EP 2004-741432	20040322
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
BR 2004008601	A	20060307	BR 2004-8601	20040322
CN 1756757	A	20060405	CN 2004-80005591	20040322
JP 2006523198	T	20061012	JP 2006-505479	20040322
NO 2005004898	A	20051024	NO 2005-4898	20051024
IN 2005CN02757	A	20070525	IN 2005-CN2757	20051024
US 2007027137	A1	20070201	US 2006-550483 IT 2003-MI573	20060616 A 20030324
PRIORITY APPLN. INFO.:			WO 2004-EP50339	W 20040322

OTHER SOURCE(S): CASREACT 141:332191; MARPAT 141:332191

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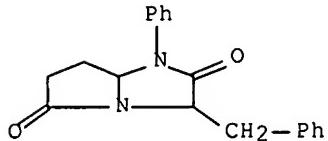


AB The title compds. [I; A = aryl, heteroaryl, arylalkyl; R1 = H, arylalkyl, heterocyclalkyl, etc.; R2 = H, alkyl, arylalkyl, Ph; or R1 and R2, taken together, form a saturated carbocyclic ring; R3 = H, alkyl, aryl, arylalkyl, heterocyclyl; n = 2-4; R4 = H, alkyl, aryl, etc.] having nootropic action (i.e., protecting and stimulating cerebral functions), analgesic action and antihyperalgesic action, and therefore useful for the treatment of cognitive deficits, and of various types of pain, were prepared. Thus, reacting tetrahydro-pyrrolo[1,2-a]imidazole-2,5-dione with iodobenzene afforded 1-phenyl-tetrahydro-1H-pyrrolo[1,2-a]imidazole-2,5-dione which was evaluated in a rat model of mononeuropathy (data given). The pharmaceutical compns. comprising the compound I are claimed.

IT 770731-04-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

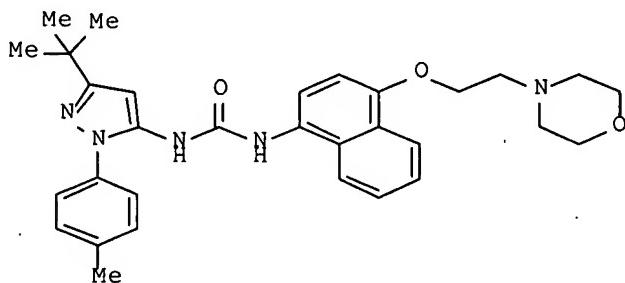
(preparation of pyrroloimidazolones with nootropic action)
RN 770731-04-9 ZCPLUS
CN 1H-Pyrrolo[1,2-a]imidazole-2,5(3H,6H)-dione, dihydro-1-phenyl-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



L34 ANSWER 10 OF 21 ZCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:142968 ZCPLUS Full-text
DOCUMENT NUMBER: 140:193056
TITLE: Combinations of active agents with p38 MAP kinase inhibitors, pharmaceutical compositions, and use in the treatment of cytokine-mediated diseases
INVENTOR(S): Simianer, Stefan; Bilbault, Pascal; Cappola, Michael L.; Way, Susan Lynn
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA;
Boehringer Ingelheim France
SOURCE: PCT Int. Appl., 168 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004014387	A1	20040219	WO 2003-US25341	20030812
· W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004110755	A1	20040610	US 2003-638702	20030811
CA 2497448	A1	20040219	CA 2003-2497448	20030812
AU 2003256410	A1	20040225	AU 2003-256410	20030812
EP 1530477	A1	20050518	EP 2003-785255	20030812
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006501218	T	20060112	JP 2004-528105	20030812
US 2007099832	A1	20070503	US 2006-539376	20061006
PRIORITY APPLN. INFO.:			US 2002-403115P	P 20020813
			US 2003-638702	B1 20030811
			WO 2003-US25341	W 20030812

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I

AB The invention relates to pharmaceutical combination therapies based on p38 kinase inhibitors and another active ingredients, pharmaceutical compns. comprising such combinations, processes for preparing them, and their use in the treatment of cytokine-mediated diseases. Preparation of I (BIRB 796 BS) is described.

IT 321656-57-9

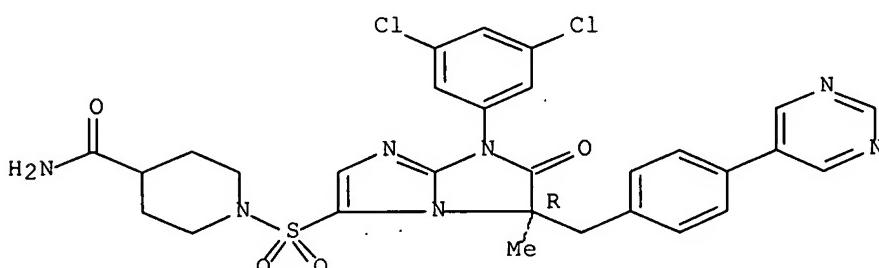
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(combinations of active agents with p38 MAP kinase inhibitors, pharmaceutical compns., and use in treatment of cytokine-mediated diseases)

RN 321656-57-9 ZCPLUS

CN 4-Piperidinecarboxamide, 1-[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 11 OF 21 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:597593 ZCPLUS Full-text

DOCUMENT NUMBER: 139:276851

TITLE: Regiocontrolled synthesis of highly-functionalized fused imidazoles: a novel synthesis of second generation LFA-1 inhibitors

AUTHOR(S): Frutos, Rogelio P.; Johnson, Michael

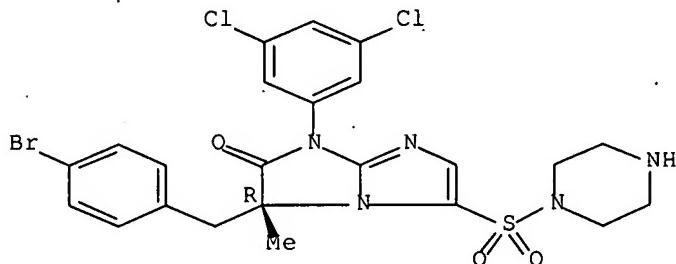
CORPORATE SOURCE: Department of Chemical Development, Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT,

SOURCE: 06877-0368, USA
 Tetrahedron Letters (2003), 44(34), 6509-6511
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 139:276851
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

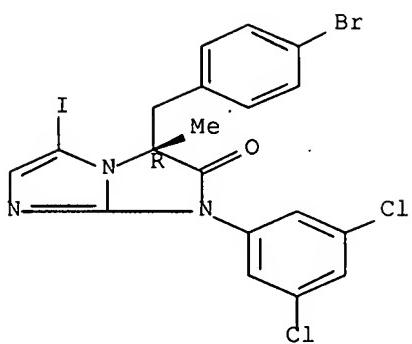
- AB A new and reliable route to a new class of LFA-1 inhibitors such as I has been developed. A key aspect of this route is the transformation of amino amide II into iodide III in four steps. Iodide III is a key advanced intermediate used in the synthesis of all second-generation 1H-imidazo[1,2-a]imidazol-2-one LFA-1 inhibitors.
- IT 321656-61-5P 321656-73-9P 397329-88-3P
 397329-89-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (regiocontrolled synthesis of fused imidazoles)
- RN 321656-61-5 ZCPLUS
- CN Piperazine, 1-[(3R)-3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



- RN 321656-73-9 ZCPLUS
- CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-5-iodo-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

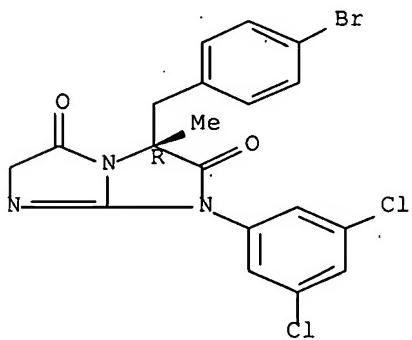
Absolute stereochemistry.



RN 397329-88-3 ZCAPLUS

CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

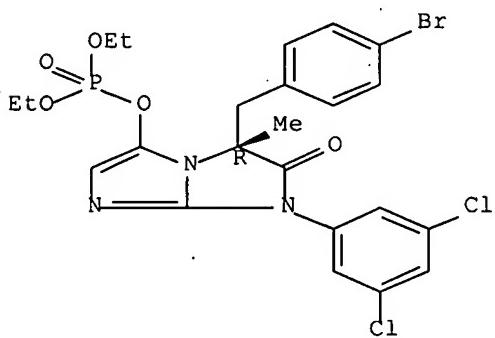
Absolute stereochemistry.



RN 397329-89-4 ZCAPLUS

CN Phosphoric acid, (3R)-3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



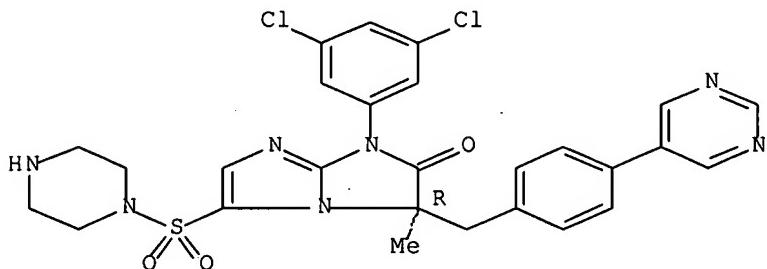
IT 321656-63-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(regiocontrolled synthesis of fused imidazoles)

RN 321656-63-7 ZCPLUS

CN Piperazine, 1-[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry...



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 12 OF 21 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:452282 ZCPLUS Full-text

DOCUMENT NUMBER: 137:169459

TITLE: Syntheses of Optically Active Tetrahydro-1H-pyrrolo[1,2-a]imidazol-2-ones and Hexahydroimidazo[1,2-a]pyridin-2(3H)-ones

AUTHOR(S): Katritzky, Alan R.; He, Hai-Ying; Wang, Jing

CORPORATE SOURCE: Center for Heterocyclic Compounds, Department of Chemistry, University of Florida, Gainesville, FL, 32611-7200, USA

SOURCE: Journal of Organic Chemistry (2002), 67(14), 4951-4956
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:169459

AB The reactions of (2S)-2-amino-2-substituted-N-(4-nitrophenyl)acetamides, succindialdehyde, and benzotriazole afforded enantiopure (3S,5R,7aR)-5-(1H-1,2,3-benzotriazol-1-yl)-3-substituted-1-(4-nitrophenyl)tetrahydro-1H-pyrrolo[1,2-a]imidazol-2-ones, which were converted by sodium borohydride into (3S,7aR)-3-substituted-1-(4-nitrophenyl)tetrahydro-1H-pyrrolo[1,2-a]imidazol-2-ones. Chiral (2S)-2-amino-2-substituted-N-(4-methylphenyl)acetamides, easily prepared in two steps from N-Boc- α -amino acids, similarly reacted with glutaraldehyde and benzotriazole to generate 5-benzotriazolyl-3-substituted-hexahydroimidazo[1,2-a]pyridin-2(3H)-ones, which were converted by sodium borohydride directly into optically active 3-substituted-hexahydroimidazo[1,2-a]pyridin-2(3H)-ones.

IT 447462-63-7P

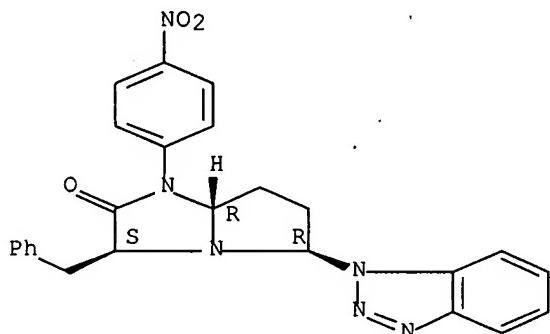
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(syntheses of optically active tetrahydro-1H-pyrrolo[1,2-a]imidazol-2-ones and hexahydroimidazo[1,2-a]pyridin-2(3H)-ones)

RN 447462-63-7 ZCPLUS

CN 1H-Pyrrolo[1,2-a]imidazol-2(3H)-one, 5-(1H-benzotriazol-1-yl)tetrahydro-1-(4-nitrophenyl)-3-(phenylmethyl)-, (3S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



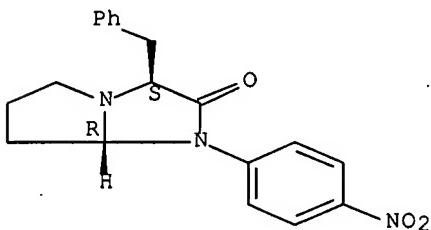
IT 447462-71-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(syntheses of optically active tetrahydro-1H-pyrrolo[1,2-a]imidazol-2-ones and hexahydroimidazo[1,2-a]pyridin-2(3H)-ones)

RN 447462-71-7 ZCPLUS

CN 1H-Pyrrolo[1,2-a]imidazol-2(3H)-one, tetrahydro-1-(4-nitrophenyl)-3-(phenylmethyl)-, (3S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 13 OF 21 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:123008 ZCPLUS Full-text

DOCUMENT NUMBER: 136:167376

TITLE: Novel preparation of (R)-3-(4-bromobenzyl)-1-(3,5-dichlorophenyl)-5-iodo-3-methyl-1H-imidazo[1,2-a]imidazol-2-one, an intermediate for antiinflammatory agents and immunomodulators

INVENTOR(S): Frutos, Rogelio P.; Johnson, Michael Dale

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 32 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002012243	A2	20020214	WO 2001-US23996	20010731
WO 2002012243	A3	20020620		
W: CA, JP, MX				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
CA 2416906	A1	20020214	CA 2001-2416906	20010731
US 2002028949	A1	20020307	US 2001-918915	20010731
US 6414161	B2	20020702		
EP 1309595	A2	20030514	EP 2001-957358	20010731
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
JP 2004505978	T	20040226	JP 2002-518218	20010731
US 2002072615	A1	20020613	US 2002-76829	20020215
US 6433183	B2	20020813		
US 2002072610	A1	20020613	US 2002-77045	20020215
US 6441183	B2	20020827		
US 2002082441	A1	20020627	US 2002-77044	20020215
US 6458986	B2	20021001		
US 2002087009	A1	20020704	US 2002-77043	20020215
US 6437148	B2	20020820		
PRIORITY APPLN. INFO.:			US 2000-224166P	P 20000809
			US 2001-918915	A3 20010731
			WO 2001-US23996	W 20010731

OTHER SOURCE(S): CASREACT 136:167376; MARPAT 136:167376
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

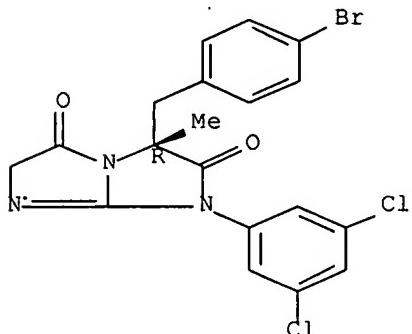
AB A novel process for the preparation of (R)-3-(4-bromobenzyl)-1-(3,5-dichlorophenyl)-5-iodo-3-methyl-1H-imidazo[1,2-a]imidazol-2-one I is disclosed. I is useful as an intermediate in the preparation of certain small mols. that are useful in the treatment or prevention of inflammatory and immune cell-mediated diseases. The invention also relates to certain intermediates used in the process. Cyclization of amino amide II with an isocyanatoacetate ester RO₂CCH₂NCO [R = C₁-6 alkyl] using a triarylphosphine, a carbon tetrahalide, and a tertiary amine, gives III. Optional alkaline hydrolysis of the resultant imidazolidinone ester III gives the acid III [R = H]. Cyclization of III [R = C₁-6 alkyl] using a Lewis acid and a phosphine oxide, or cyclization of III [R = H] using a coupling agent, gives dione IV. Reaction of IV with a strong base and a chlorophosphate (R'O)₂POCl gives an enol phosphate V, which is iodinated with Me₃SiI or NaI/Me₃SiCl to give I. In a specific example using R = R' = Et, a yield of 89% was obtained in the key cyclization of III (AlMe₃ and Ph₃PO), and 69% was obtained in the final iodination step (NaI/Me₃SiCl).

IT 397329-88-3P, (3R)-(4-Bromobenzyl)-1-(3,5-dichlorophenyl)-3-methyl-1,6-dihydroimidazo[1,2-a]imidazole-2,5-dione 397329-89-4P, Phosphoric acid (3R)-5-(4-bromobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl diethyl ester
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1H-imidazo[1,2-a]imidazol-2-one derivative as intermediate for immunomodulators and antiinflammatory agents)

RN 397329-88-3 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

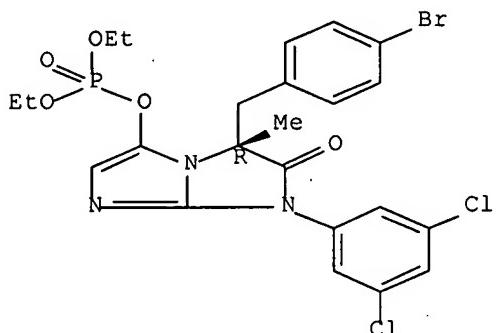
Absolute stereochemistry.



RN 397329-89-4 ZCPLUS

CN Phosphoric acid, (3R)-3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 321656-73-9P, (3R)-(4-Bromobenzyl)-1-(3,5-dichlorophenyl)-5-iodo-3-methyl-1H-imidazo[1,2-a]imidazol-2-one

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of 1H-imidazo[1,2-a]imidazol-2-one derivative as intermediate

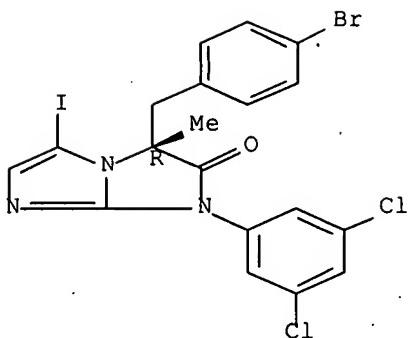
for

immunomodulators and antiinflammatory agents)

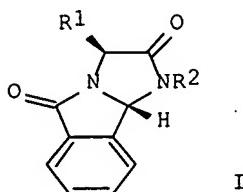
RN 321656-73-9 ZCPLUS

CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-5-iodo-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



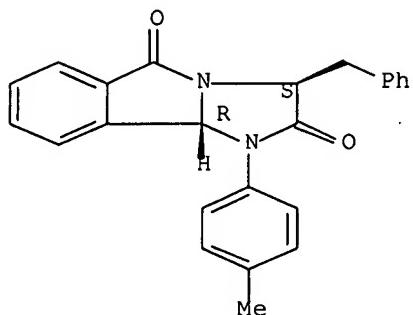
L34 ANSWER 14 OF 21 ZCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2001:541387 ZCPLUS Full-text
 DOCUMENT NUMBER: 135:357878
 TITLE: Stereoselective syntheses of 1H-imidazo[2,1-a]isoindole-2,5(3H,9bH)-diones
 AUTHOR(S): Katritzky, Alan R.; Xu, Yong-Jiang; He, Hai-Ying;
 Steel, Peter J.
 CORPORATE SOURCE: Center for Heterocyclic Chemistry, Department of
 Chemistry, University of Florida, Gainesville, FL,
 32611-7200, USA
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1
 (2001), (15), 1767-1770
 CODEN: JCSPCE; ISSN: 1472-7781
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 135:357878
 GI



- AB Title imidazoisoindolediones I (R1 = MeCH₂CHMe, Me, Me₂CH, benzyl; R2 = 4-MeC₆H₄, Ph, 4-FC₆H₄, Bu, cyclohexyl) were prepared in 67-96% yields with high stereoselectivities via intermol. condensation of 2-formylbenzoic acid and α -amino amides R₁CH(NH₂)CONHR₂ in the presence of a catalytic amount of p-toluenesulfonic acid. Intermediate α -amino amides R₁CH(NH₂)CONHR₂ were obtained in two steps from easily available chiral N-Boc- α -amino acids.
- IT 372187-77-4P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (crystal structure of imidazoisoindoledione prepared via
 cyclocondensation of formylbenzoic acid with amino acid amides)
- RN 372187-77-4 ZCPLUS

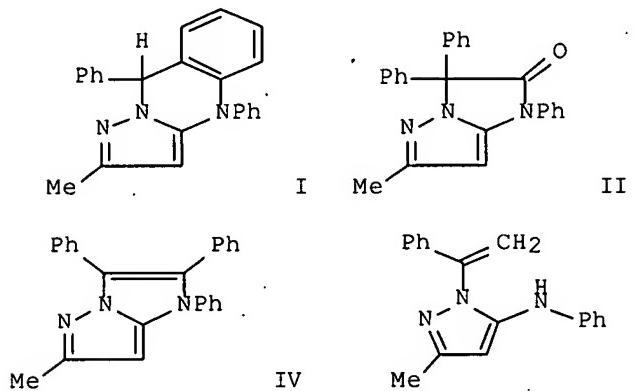
CN 1H-Imidazo[2,1-a]isoindole-2,5(3H,9bH)-dione, 1-(4-methylphenyl)-3-(phenylmethyl)-, (3S,9bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 15 OF 21 ZCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:68049 ZCPLUS Full-text
DOCUMENT NUMBER: 128:154055
TITLE: Synthesis of pyrazolo-fused heterocycles by a tandem Appel's dehydration/electrocyclization methodology
AUTHOR(S): Lee, Kee-Jung; Kwon, Heung-Taeck; Kim, Boo-Geun
CORPORATE SOURCE: Department of Industrial Chemistry, Hanyang University, Seoul, 133-791, S. Korea
SOURCE: Journal of Heterocyclic Chemistry (1997), 34(6), 1795-1799
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



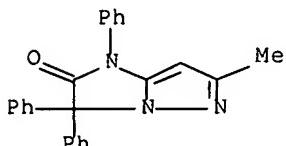
AB The hydrazones of benzophenone, benzil, and acetophenone were allowed to react with acetoacetanilide to give azinoamides PhCR:NN:CMeCH₂CONHPh (I, R = Ph, COPh, Me), and the reaction of I with Appel's dehydration conditions (triphenylphosphine/carbon tetrachloride/triethylamine) led to the corresponding azinoketimines, which underwent electrocyclic ring closure under the reaction conditions to give pyrazolo-fused heterocycles. Azinoamide I (R = Ph) gave a 4,9-dihydropyrazolo[5,1-b]quinazoline II, while I (R = COPh) yielded 2,3-dihydro-1H-imidazo[1,2-b]pyrazol-2-one III and 1H-imidazo[1,2-b]pyrazole IV. I (R = Me) gave a monocyclic N- α -styryl-5-(phenylamino)pyrazole V.

IT 202481-62-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrazolo-fused heterocycles by Appel's
dehydration/electrocyclization of hydrazones)

RN 202481-62-7 ZCPLUS

CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 6-methyl-1,3,3-triphenyl- (9CI) (CA
INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 16 OF 21 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1987:196519 ZCPLUS Full-text
DOCUMENT NUMBER: 106:196519

TITLE: Reactions of azines. 12. Preparation and reactions of triphenyl[2-([phenyl(methoxycarbonyl)methylene]hydrazono)propyl]phosphonium bromide

AUTHOR(S): Schweizer, E. E.; Hayes, J. E.; Rheingold, A.; Xu, Wei
CORPORATE SOURCE: Dep. Chem., Univ. Delaware, Newark, DE, 19716, USA
SOURCE: Journal of Organic Chemistry (1987), 52(9), 1810-16

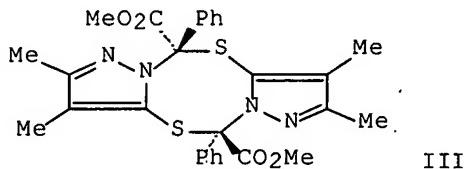
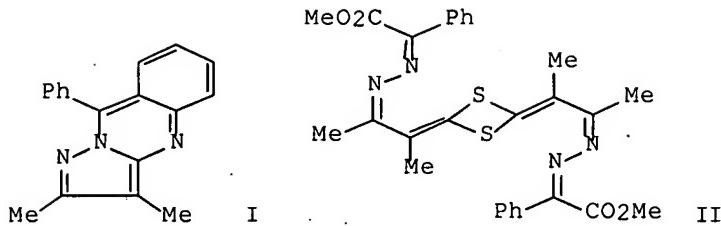
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

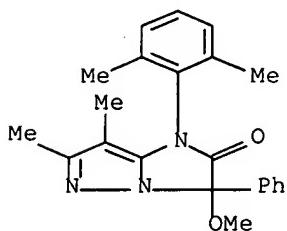
LANGUAGE: English

OTHER SOURCE(S): CASREACT 106:196519

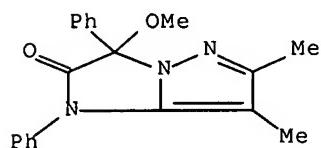
GI



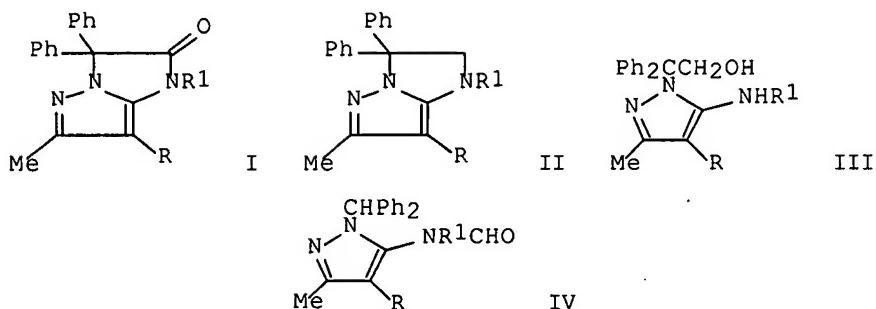
AB Ph(MeO₂C)C:NN:CMeCHRP+Ph₃X- (R = H, X = Br; R = Me, X = iodide) and their ylides Ph(MeO₂C)C:NN:CMeCR:PPh₃ were prepared and their reactions to give, e.g., pyrazoloquinazoline I, desaurine (II), and dipyrazolodiazadithiocine III are described. The crystal structures of I-III were determined
 IT 107769-80-2P 107769-81-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 107769-80-2 ZCAPLUS
 CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 1-(2,6-dimethylphenyl)-3-méthoxy-6,7-dimethyl-3-phenyl- (9CI) (CA INDEX NAME)



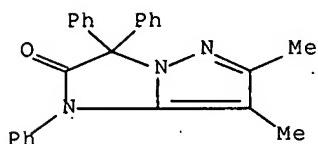
RN 107769-81-3 ZCAPLUS
 CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 3-methoxy-6,7-dimethyl-1,3-diphenyl- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1985:6313 ZCPLUS Full-text
 DOCUMENT NUMBER: 102:6313
 TITLE: Novel lithium aluminum hydride reduction pathway.
 Reactions of 2,3-dihydro-1H-imidazo[1,2-b]pyrazol-2-ones with lithium aluminum hydride. Preparations of 2,3-dihydro-1H-imidazo[1,2-b]pyrazoles and side products
 AUTHOR(S): Schweizer, Edward E.; Lee, Kee Jung
 CORPORATE SOURCE: Dep. Chem., Univ. Delaware, Newark, DE, 19711, USA
 SOURCE: Journal of Organic Chemistry (1984), 49(25), 4848-53
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 102:6313
 GI

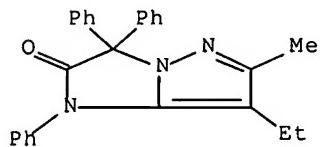


- AB The direct LiAlH₄ reduction of 2,3-dihydro-1H-imidazo[1,2-b]pyrazol-2-ones (I) to 2,3-dihydro-1H-imidazo[1,2-b]pyrazoles (II) was unsuccessful. Reduction of I (R, R1 = Me, Ph; Et, Ph; Me, 4-MeOC₆H₄; Et, 4-F₃CC₆H₄) gave an N-carbonyl cleavage followed by carbonyl reduction to amino alcs. III. Reduction of I (R, R1 = Me, Me₃C; allyl, Me₃C; Me, Me; allyl, Me) gave an unusual formamide product, IV, further LiAlH₄ treatment of which gave II. Dehydrative ring closure of compds. III (R = Me, Et; R1 = Ph) with P₂O₅ gave the corresponding II.
 IT 89726-11-4 89726-13-6 89726-25-0
 89726-36-3 92816-79-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reduction of, with lithium aluminum hydride)
 RN 89726-11-4 ZCPLUS
 CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 6,7-dimethyl-1,3,3-triphenyl- (9CI)
 (CA INDEX NAME)



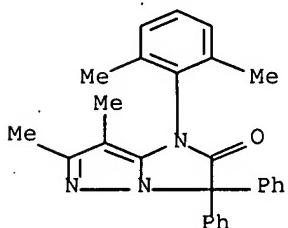
RN 89726-13-6 ZCPLUS

CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 7-ethyl-6-methyl-1,3,3-triphenyl-
(9CI) (CA INDEX NAME)



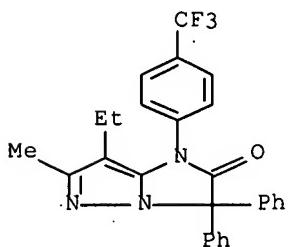
RN 89726-25-0 ZCPLUS

CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 1-(2,6-dimethylphenyl)-6,7-dimethyl-
3,3-diphenyl- (9CI) (CA INDEX NAME)



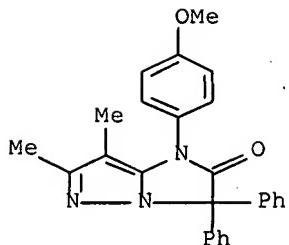
RN 89726-36-3 ZCPLUS

CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 7-ethyl-6-methyl-3,3-diphenyl-1-[4-
(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

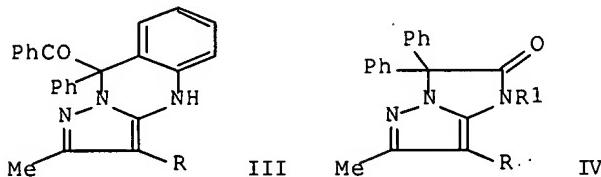


RN 92816-79-0 ZCPLUS

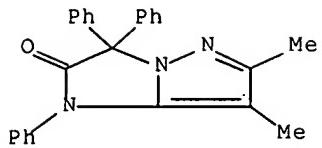
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 1-(4-methoxyphenyl)-6,7-dimethyl-3-
diphenyl- (9CI) (CA INDEX NAME)



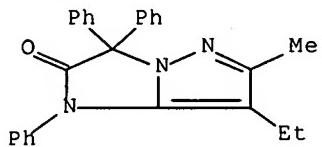
L34 ANSWER 18 OF 21 ZCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1984:209740 ZCPLUS Full-text
 DOCUMENT NUMBER: 100:209740
 TITLE: Reactions of azines. 9. Rearrangement of 1-oxo-3,4,8-triaza-2,4,6,7-octatetraenes to 2,3-dihydro-1H-imidazo[1,2-b]pyrazol-2-ones and 4,9-dihydropyrazolo[5,1-b]quinazolines
 AUTHOR(S): Schweizer, Edward E.; Lee, Kee Jung
 CORPORATE SOURCE: Dep. Chem., Univ. Delaware, Newark, DE, 19711, USA
 SOURCE: Journal of Organic Chemistry (1984), 49(11), 1964-9
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 100:209740
 GI



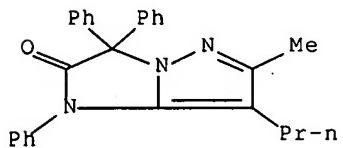
- AB The reactions of PhCOPh:NN:CMeCR:X (I; R = Me, Et, Pr, allyl, PhCH₂; X = PPh₃) with R₁NCO (II; R₁ = Me, Me₃C, Ph, substituted Ph, etc.) gave the title heterocycles III and IV, presumably via I (X = C:NR₁). The III:IV ratio increased with increasing bulk of R and R₁ and decreased linearly with increasing σ_P value of the substituents in II [R₁ = (un)substituted phenyl]: $\rho = -0.5$. The III:IV ratios obtained from I (R = Et) and undistd. II were .apprx.65:35, reversed compared to the results obtained with freshly distilled II.
- IT 89726-11-4P 89726-13-6P 89726-15-8P
 89726-17-0P 89726-18-1P 89726-20-5P
 89726-22-7P 89726-24-9P 89726-25-0P
 89726-31-8P 89726-33-0P 89726-35-2P
 89726-36-3P 89726-37-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
- RN 89726-11-4 ZCPLUS
- CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 6,7-dimethyl-1,3,3-triphenyl- (9CI)
 (CA INDEX NAME)



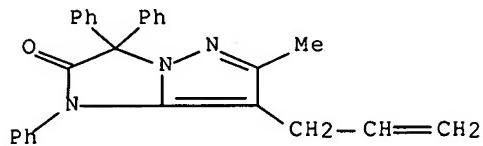
RN 89726-13-6 ZCPLUS
 CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 7-ethyl-6-methyl-1,3,3-triphenyl- (9CI) (CA INDEX NAME)



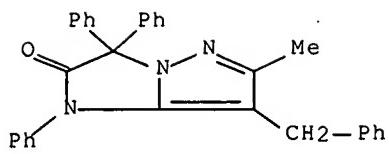
RN 89726-15-8 ZCPLUS
 CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 6-methyl-1,3,3-triphenyl-7-propyl- (9CI) (CA INDEX NAME)



RN 89726-17-0 ZCPLUS
 CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 6-methyl-1,3,3-triphenyl-7-(2-propenyl)- (9CI) (CA INDEX NAME)

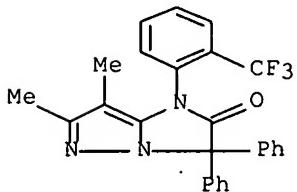


RN 89726-18-1 ZCPLUS
 CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 6-methyl-1,3,3-triphenyl-7-(phenylmethyl)- (9CI) (CA INDEX NAME)



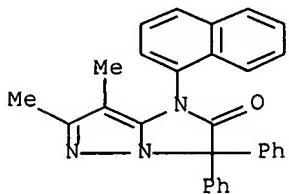
RN 89726-20-5 ZCPLUS

CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 6,7-dimethyl-3,3-diphenyl-1-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



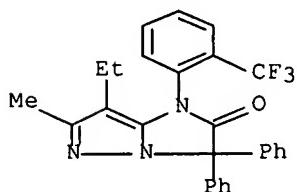
RN 89726-22-7 ZCPLUS

CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 6,7-dimethyl-1-(1-naphthalenyl)-3,3-diphenyl- (9CI) (CA INDEX NAME)



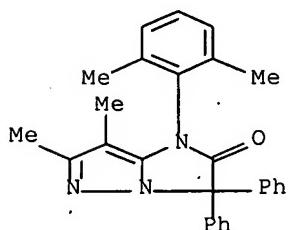
RN 89726-24-9 ZCPLUS

CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 7-ethyl-6-methyl-3,3-diphenyl-1-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



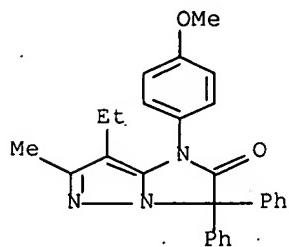
RN 89726-25-0 ZCPLUS

CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 1-(2,6-dimethylphenyl)-6,7-dimethyl-3,3-diphenyl- (9CI) (CA INDEX NAME)



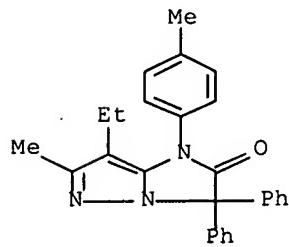
RN 89726-31-8 ZCPLUS

CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 7-ethyl-1-(4-methoxyphenyl)-6-methyl-3,3-diphenyl- (9CI) (CA INDEX NAME)



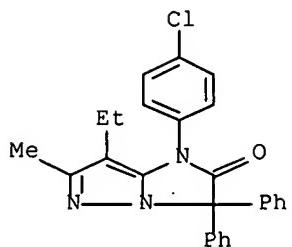
RN 89726-33-0 ZCPLUS

CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 7-ethyl-6-methyl-1-(4-methylphenyl)-3,3-diphenyl- (9CI) (CA INDEX NAME)

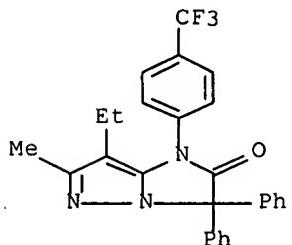


RN 89726-35-2 ZCPLUS

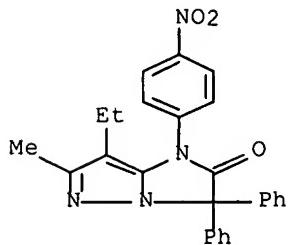
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 1-(4-chlorophenyl)-7-ethyl-6-methyl-3,3-diphenyl- (9CI) (CA INDEX NAME)



RN 89726-36-3 ZCPLUS
 CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 7-ethyl-6-methyl-3,3-diphenyl-1-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 89726-37-4 ZCPLUS
 CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 7-ethyl-6-methyl-1-(4-nitrophenyl)-3,3-diphenyl- (9CI) (CA INDEX NAME)



L34 ANSWER 19 OF 21 ZCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1984:201300 ZCPLUS Full-text
 DOCUMENT NUMBER: 100:201300
 TITLE: The structures of 3-allyl-9-benzoyl-2-methyl-9-phenyl-4,9-dihdropyrazolo[5,1-b]quinazoline, C₂₇H₂₃N₃O, and 6,7-dimethyl-1,3,3-triphenyl-1H-imidazo[1,2-b]pyrazol-2(3H)-one, C₂₅H₂₁N₃O
 AUTHOR(S): Rheingold, A. L.; Fultz, W. C.; Schweizer, E. E.; Lee, K. J.
 CORPORATE SOURCE: Dep. Chem., Univ. Delaware, Newark, DE, 19716, USA
 SOURCE: Acta Crystallographica, Section C: Crystal Structure

Communications (1984), C40(4), 687-90
CODEN: ACSCEE; ISSN: 0108-2701

DOCUMENT TYPE: Journal
LANGUAGE: English

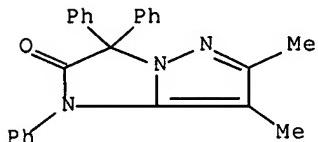
AB C₂₇H₂₃N₃O is orthorhombic, space group Pbcs, with a 13.025(4), b 15.99(3)°, and c 20.593(6) Å at 297 K; d.(calculated) = 1.26 for Z = 8; R for 1671 unique reflections [I ≥ 2σ(I)] = 0.0728, C₂₅H₂₁N₃O is, monoclinic, space group P21/c, with a 11.234(4), b 7.021(1), c 25.330(6) Å, and β 91.83(3)° at 299 K; d.(calculated) = 1.26 for Z = 4. R for 1383 unique reflections [I ≥ 2.75 σ (I)] = 0.0770. Atomic parameters are given. Bond distances and angles are all within the expected ranges. The 1,2-diazacyclopentadiene rings in both structures are nearly planar.

IT 89726-11-4

RL: PRP (Properties)
(crystal structure of)

RN 89726-11-4 ZCPLUS

CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 6,7-dimethyl-1,3,3-triphenyl- (9CI)
(CA INDEX NAME)



L34 ANSWER 20 OF 21 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1980:22339 ZCPLUS Full-text

DOCUMENT NUMBER: 92:22339

TITLE: Reactions of ketenimines with nitrones

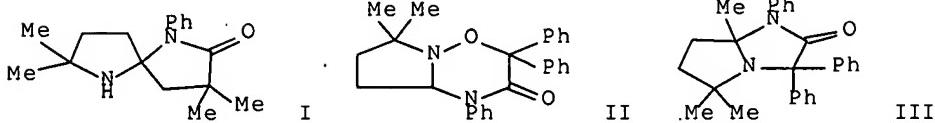
AUTHOR(S): Tsuge, Otohiko; Watanabe, Hiroyuki; Masuda, Kichiro;
Yousif, Mohamed M.

CORPORATE SOURCE: Res. Inst. Ind. Sci., Kyushu Univ., Fukuoka, 812,
Japan

SOURCE: Journal of Organic Chemistry (1979), 44(25), 4543-7
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal
LANGUAGE: English

GI



AB Dimethylketene-N-phenylimine reacts with benzylidenaniline N-oxides and cinnamylidenaniline N-oxide to give the corresponding 1:1 adducts, 1-[o-

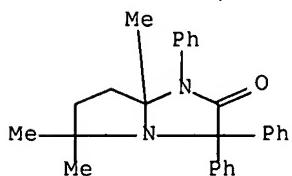
(benzylidenamino)phenyl]-1,1-dimethylacetanilides, which are easily hydrolyzed to 3,3-dimethyloxindole, whereas the reaction of the ketenimine with cyclic nitrones such as 1-pyrroline 1-oxides afforded 1:1 adducts, imidazolidinone and (or) diazaspiro[4.4]nonanone derivative I. In the reaction of diphenylketene-N-phenylimine with cyclic nitrones, a perhydropyrrooxadiazinone II or imidazolidinone III is formed, depending on the nature of cyclic nitrones.

IT 71871-89-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 71871-89-1 ZCPLUS

CN 1H-Pyrrolo[1,2-a]imidazol-2(3H)-one, tetrahydro-5,5,7a-trimethyl-1,3,3-triphenyl- (9CI) (CA INDEX NAME)



L34 ANSWER 21 OF 21 ZCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1977:5414 ZCPLUS Full-text

DOCUMENT NUMBER: 86:5414

TITLE: Synthesis of imidazolino[1,2-f]xanthin-2-ones and their derivatives substituted at the methylene group

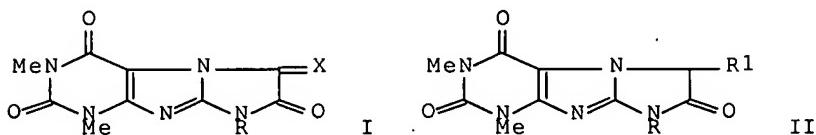
AUTHOR(S): Nosachenko, V. I.; Kochergin, P. M.; Steblyuk, P. N.
CORPORATE SOURCE: Zaporozh. Med. Inst., Zaporozhe, USSR

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1976), (8), 1132-5

DOCUMENT TYPE: CODEN: KGSSAQ; ISSN: 0132-6244

LANGUAGE: Journal

GI Russian



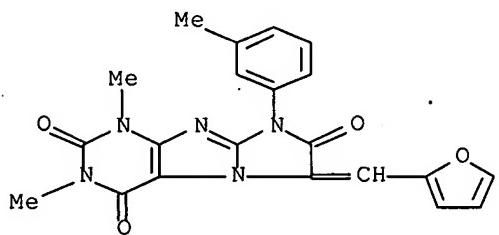
AB Imidazoloxanthinones (I, R = H, Ph, m-MeC₆H₄, X = H₂) were obtained in 70-80% yields from the appropriate theophylline by treatment with a haloacetate followed by cyclization. Condensation of I with aldehydes and ketones gave 50-94% I (X = PhCH, p-Me₂NC₆H₄CH, PhCH:CHCH, Me₂CH, furfurylidene, isatin residue). Addnl. obtained were I (X = p-Me₂NC₆H₄N) and II (R1 = PhN:N, p-H₂NSO₂C₆H₄N:N, p-MeOC₆H₄N:N).

IT 61034-26-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 61034-26-2 ZCPLUS

CN 1H-Imidazo[2,1-f]purine-2,4,7(3H,6H,8H)-trione, 6-(2-furanylmethylene)-1,3-dimethyl-8-(3-methylphenyl)- (9CI) (CA INDEX NAME)



=> d his full

(FILE 'HOME' ENTERED AT 10:11:22 ON 27 JUN 2007)

FILE 'REGISTRY' ENTERED AT 10:12:05 ON 27 JUN 2007

L1 STRUCTURE UPLOADED
L2 27 SEA SSS SAM L1
D STAT QUE L2

FILE 'ZCPLUS' ENTERED AT 10:16:34 ON 27 JUN 2007

L3 12 SEA ABB=ON PLU=ON L2
L4 22734 SEA ABB=ON PLU=ON WU J?/AU
L5 1187 SEA ABB=ON PLU=ON KELLY T?/AU
L6 419 SEA ABB=ON PLU=ON LEMIEUX R?/AU
L7 1095 SEA ABB=ON PLU=ON GOLDBERG D?/AU
L8 8 SEA ABB=ON PLU=ON EMEIGH J?/AU
E EMEIGH/AU
L9 21 SEA ABB=ON PLU=ON SORCEK R?/AU
L10 16 SEA ABB=ON PLU=ON L4 AND (L5 OR L6 OR L7 OR L8 OR L9)
L11 11 SEA ABB=ON PLU=ON L5 AND (L6 OR L7 OR L8 OR L9)
L12 2 SEA ABB=ON PLU=ON L6 AND (L7 OR L8 OR L9)
L13 2 SEA ABB=ON PLU=ON L7 AND (L8 OR L9)
L14 3 SEA ABB=ON PLU=ON L8 AND L9
L15 22 SEA ABB=ON PLU=ON (L10 OR L11 OR L12 OR L13 OR L14)
L16 4 SEA ABB=ON PLU=ON L3 AND (L4 OR L5 OR L6 OR L7 OR L8 OR L9)

FILE 'REGISTRY' ENTERED AT 10:24:37 ON 27 JUN 2007

L17 24 SEA ABB=ON PLU=ON L2 AND CL>0

FILE 'ZCPLUS' ENTERED AT 10:24:52 ON 27 JUN 2007

L18 4 SEA ABB=ON PLU=ON L17 AND L16

FILE 'REGISTRY' ENTERED AT 10:25:59 ON 27 JUN 2007

L19 572 SEA SSS FUL L1
SAVE TEMP L19 WAR412STR1L/A

FILE 'ZCPLUS' ENTERED AT 10:26:41 ON 27 JUN 2007

L20 28 SEA ABB=ON PLU=ON L19

FILE 'REGISTRY' ENTERED AT 10:27:37 ON 27 JUN 2007

L21 0 SEA ABB=ON PLU=ON (L4 OR L5 OR L6 OR L7 OR L8 OR L9) AND L20

FILE 'ZCPLUS' ENTERED AT 10:28:41 ON 27 JUN 2007

L22 7 SEA ABB=ON PLU=ON (L4 OR L5 OR L6 OR L7 OR L8 OR L9) AND L20

L23 23 SEA ABB=ON PLU=ON L15 OR L22

FILE 'REGISTRY' ENTERED AT 10:29:28 ON 27 JUN 2007

L24 FILE 'ZCPLUS' ENTERED AT 10:32:32 ON 27 JUN 2007
21 SEA ABB=ON PLU=ON L20 NOT L23
D SCA
D SCA L22

FILE 'REGISTRY' ENTERED AT 10:36:30 ON 27 JUN 2007

L25 284 SEA ABB=ON PLU=ON L19 AND CL>1 AND BR>0
L26 210 SEA ABB=ON PLU=ON L25 AND N>3

L27 201 SEA ABB=ON PLU=ON L26 AND O>1
L28 0 SEA ABB=ON PLU=ON L27 AND NC>1
L29 32 SEA ABB=ON PLU=ON L27 AND 3/NRS
 D SCA
L30 125 SEA ABB=ON PLU=ON L27 AND 4/NRS
L31 43 SEA ABB=ON PLU=ON L27 AND 5/NRS
L32 200 SEA ABB=ON PLU=ON (L29 OR L30 OR L31)
L33 1 SEA ABB=ON PLU=ON L27 NOT L32
 D SCA
 D SCA L30

FILE 'REGISTRY' ENTERED AT 10:44:27 ON 27 JUN 2007

FILE 'ZCPLUS' ENTERED AT 10:44:31 ON 27 JUN 2007
D STAT QUE L20
D STAT QUE L23
D IBIB ABS HITIND L23 1-23

FILE 'REGISTRY' ENTERED AT 10:45:55 ON 27 JUN 2007

FILE 'ZCPLUS' ENTERED AT 10:45:59 ON 27 JUN 2007
D STAT QUE L20

L34 21 SEA ABB=ON PLU=ON L20 NOT L23
D IBIB ABS HITSTR L34 1-21

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 26 JUN 2007 HIGHEST RN 939408-72-7
DICTIONARY FILE UPDATES: 26 JUN 2007 HIGHEST RN 939408-72-7

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<http://www.cas.org/support/stngen/stndoc/properties.html>

FILE ZCPLUS

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FILE LAST UPDATED: 26 Jun 2007 (20070626/ED)

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